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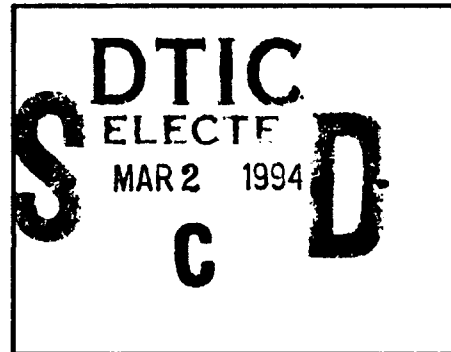
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**CRDEC-TR-144**

**A STUDY OF THE CRYSTALLIZATIONS POSSIBLE  
ON THE SURFACE OF A SPHERICAL DROPLET  
USING COULOMB INTERACTIONS  
BETWEEN POINT CHARGES**

**Burt V. Bronk, Ph.D.  
Robert H. Frickel**

**RESEARCH DIRECTORATE**

**January 1990**

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A STUDY OF THE CRYSTALLIZATIONS POSSIBLE  
ON THE SURFACE OF A SPHERICAL DROPLET  
USING COULOMB INTERACTIONS BETWEEN POINT CHARGES

## 1. INTRODUCTION

When conditions are appropriate, many pure substances can assume a crystalline form in the solid state. The exact form of the crystal that occurs is determined by the symmetries that are available and by the form of interaction between the molecules forming the crystal. If molecules constrained to the surface of a sphere condensed into a crystal, one would not expect the same geometry for the crystal as would occur for the same molecules in a three-dimensional crystal since the surface is two-dimensional. Further, since a sphere cannot be mapped onto a plane without stretching, the crystals allowed will not be identical with those which are known from studies which have been done in a plane. The possibility of such crystals is of more than theoretical interest, since it is now possible to measure the formation of layers of molecules on the surface of micron sized liquid droplets.<sup>1</sup>

In previous publications,<sup>2,3</sup> we considered the ordered configurations which result when charged particles constrained to move on the surface of a sphere relaxed to a crystalline-like order. In the CRDEC report<sup>1</sup> we presented the configurations which resulted when the number of charged particles,  $N$ , varied from between two and thirty-two as well as the individual case of  $N$  equal to thirty-six. In reference 2 we tabulated all configurations resulting from this procedure for charge number ranging from  $N = 2$  to  $N = 40$ . In that article we presented a new tetrahedral configuration as the lowest energy configuration for  $N = 16$  and presented new configurations for  $N = 19$  through 40. It should be mentioned that this problem has been of interest to physicists and mathematicians for some time and a number of the earlier results<sup>3-11</sup> are discussed in reference 2. In the present paper we extend those studies to include all the additional cases up to  $N = 108$  including more than one equilibrium configuration in some cases. From the fairly large number of configurations available, we are able to draw some conclusions about the symmetries and associated geometries. If crystallizations can be induced for molecules confined to the surface of a sphere we predict that the configurations which are actually observed will show similarities for many types of interactions between molecules to the symmetries and geometries obtained in this study.

## 2. METHODS

For the present study, we consider  $N$  point charges confined to the surface of a sphere and interacting via a three-dimensional Coulomb repulsion. The computer calculation is approximately the same as was described in our previous publications and is only briefly described here. The point charges are initially randomly placed on the sphere and are allowed to relax as though moved by the Coulomb force in a viscous fluid. They continue to move until the tangential force on any one of those point particles is negligible. The configuration obtained at this point then usually (but not always) has a symmetry apparent when nearest neighbor points are joined to form a polyhedron.

The equilibrium configuration resulting from each computation is displayed in a table in the Appendix. Each table is labeled with the number of charged points moving on the sphere and with the symmetry group of the configuration. The points are listed from top to bottom in order of their individual point energies which are also tabulated. The column labeled "index" indicates the order of the points according to their theta coordinate on the sphere and is an aid for identifying specific points on the figures. We present a number of the configurations in equal area projections (see Figures 2 to 10). The circles represent parallel circles thirty degrees apart on the sphere. Different types of lines represent edges of slightly different lengths between charged points which are nearest neighbors (See Figure 1). The perpendicular lines through the centers of the circles represent meridional great circles through the poles. Both hemispheres are seen as though looking down through a transparent half sphere.

The equal area projections were rotated into configurations which made the symmetries evident. In doing this, use was made of tabulations of individual particle energies as are given in the Appendix. It may be seen that when there are symmetries, equal energy subsets of equivalent particles occur (this is discussed further in the Results section). As an example of how this information may be used, consider the table for  $N = 40$ . Here subsets of four charges, each having equal individual particle energies occur. To obtain a configuration showing the  $D_2$  symmetry, two points relatively near each other (Index 1 and 2) were rotated so that the North pole bisected the great circle between them resulting in the configuration given in the table.

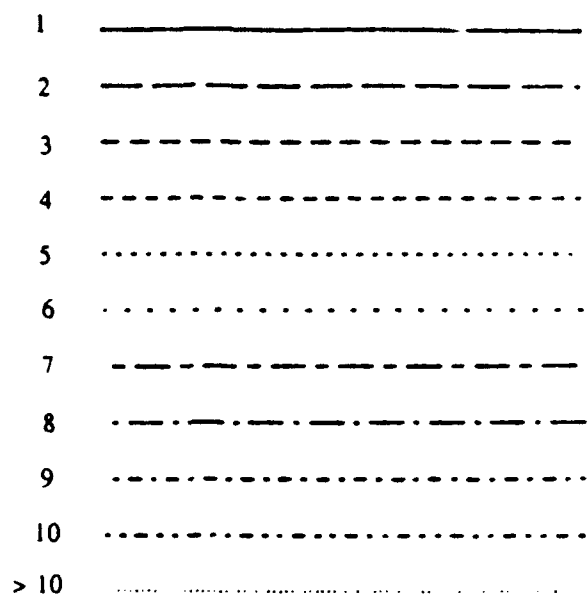


Figure 1. Representations of polyhedron edges joining neighboring points in order of increasing lengths.

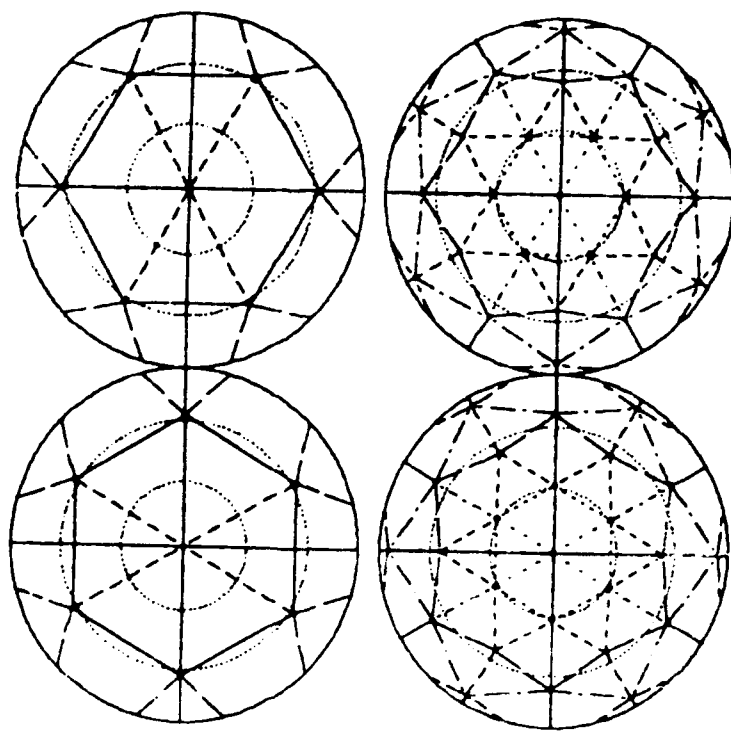


Figure 2. The two six-fold configurations with  $N = 14$  (on the left) and  $N = 50$ .

### 3. RESULTS

#### 3.1 General Observations from Table 1

The symmetries of the equilibrium configurations are summarized in Table 1. The point group classifications are listed for all charge numbers from  $N = 2$  to  $N = 108$ , so that the table includes configurations which were known prior to the present investigation as well as many new ones. In addition to the minimal energy configuration, a number of interesting higher energy configurations which we have studied are also listed. For example, for  $N = 20$ , it has been known for some time that the dodecahedron (Icosahedral symmetry) has substantially higher energy than a  $D_{3vh}$  configuration.<sup>1,2</sup>

Some general observations may be made from this table. First, we note that there are no seven-fold symmetric equilibrium configurations listed, although it was easy to construct a seven-fold unstable equilibrium figure with nine points, for example. Six-fold symmetries are also not commonplace, since only two of them have appeared up to charge number 108. We have shown the two six-fold symmetric cases in Figure 2. On the other hand five-fold rotational symmetries are rather numerous. Counting the icosahedral cases, there are nine minimal energy configurations with five-fold symmetry. Note that each of these has a charge number which fits the prescription  $N = 5n + 2$ , where  $n$  is an integer. Note however that many  $N$  satisfying this do not exhibit the five-fold symmetry. The icosahedral figures are shown in Figure 3 and the other five-fold symmetric figures are shown in Figures 4 and 5. We observe that a kind of self-similarity occurs for higher charge number in that the five pointed star at the center and equilateral pentagons at various theta are apparent in the equal-area projections.

Another point of interest is that four-fold rotational symmetry occurs only in rotation reflection or octahedral symmetries. The polyhedra for the equilibrium figures with four-fold rotational symmetry having at least one plane square face show in their projections a self-similar appearing geometry as charge number increases. This may be seen in Figure 6.

As we move higher in charge number, stretches of charge number with only two-fold symmetry occur, although at charge number 100, a tetrahedral symmetry is encountered. It appears that at low symmetry, a pure rotational symmetry is more common than a pure reflectional symmetry. This is at first surprising. However, if one rotates the configurations through various orientations one may see numerous cases where there is a local dihedral line about which one sees an approximate bilateral symmetry (common in biology) in

TABLE 1.  
Point Group Classification of Equilibrium Configurations

<u>Symmetry</u>	<u>Number of charges</u>
D <sub>∞</sub>	2
Icosahedral	12*, 32*, 72, 20*+, 30*+
Octahedral	6*, 24, 44*, 48, 8*+, 14*+
Tetrahedral	4*, 16, 22*, 28, 46, 100
D <sub>6d</sub> (S <sub>12v</sub> )	14, 50
D <sub>4d</sub> (S <sub>8v</sub> )	8, 10, 18, 80, 16+, 32+
D <sub>5vh</sub>	7, 17, 27, 42
D <sub>5</sub>	67, 77
C <sub>5v</sub>	11+
D <sub>3vh</sub>	3, 5, 9, 20, 39, 41
C <sub>3v</sub>	31, 7+
D <sub>3</sub>	15, 23, 29, 45, 51, 57, 60, 63, 69, 75, 78, 101, 102
C <sub>3</sub>	49, 52, 61+, 94+
D <sub>2</sub>	30, 34, 36, 40, 58, 64, 68, 74+, 90, 94, 104, 106
C <sub>2v</sub>	11, 13, 19, 21, 38, 43, 53
C <sub>2</sub>	26, 35, 37, 54, 55, 56, 59, 62, 63, 65, 66, 70, 71, 73, 76, 81, 82, 83, 84, 85, 86, 87, 88, 89, 91, 92, 93, 95, 96, 97, 98, 99, 103, 105+, 107, 108
C <sub>s</sub> (reflection only)	25, 33, 47, 79, 94+
C <sub>1</sub> (no symmetry)	61, 74, 105

\*with all reflection planes

+additional configuration with higher energy

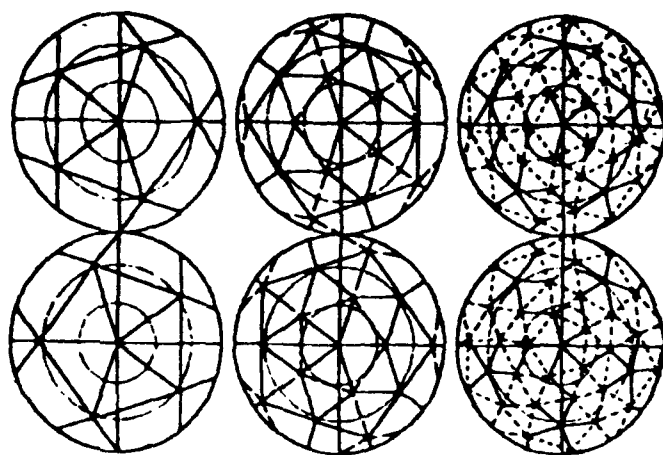


Figure 3. Equilibrium Figures with icosahedral symmetry. From the left:  $N = 12$ ;  $N = 32$ ;  $N = 72$ .

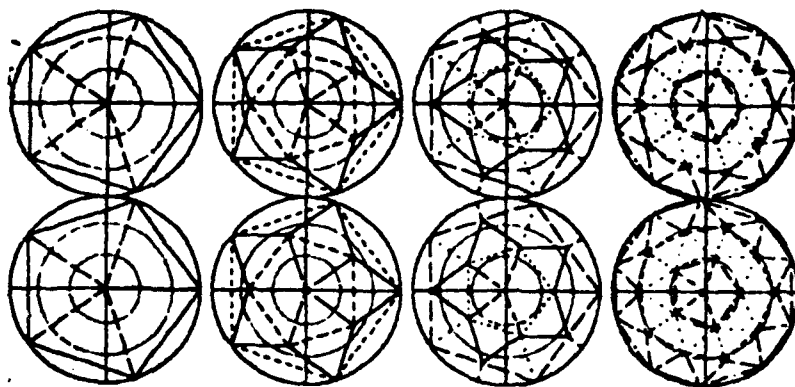


Figure 4. Equilibrium Figures with five-fold rotational symmetry and vertical and horizontal reflection planes. From the left:  $N = 7$ ;  $N = 17$ ;  $N = 27$ ;  $N = 42$ .

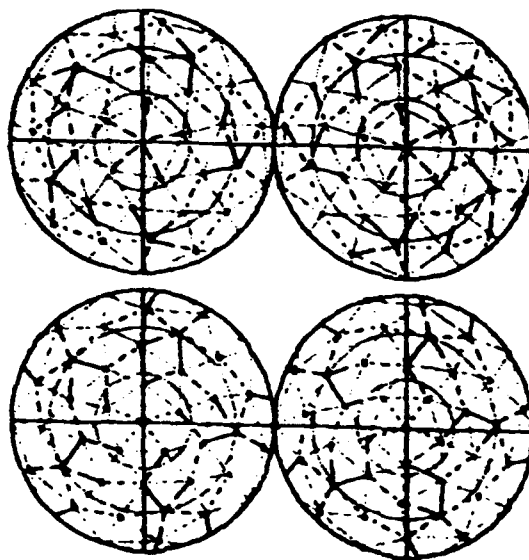


Figure 5. Equilibrium Figures with five-fold rotational symmetry and perpendicular two-fold axes, but no reflection planes.  $N = 67$  (on the left) and  $N = 77$ .

at least part of a hemisphere. Examples of this are shown for  $N = 26$  and  $N = 99$  in Figure 7.

We have come across several cases where there are two or more equilibrium figures for the same charge number. These have Coulomb energies that are very close to one another. An interesting example is found at  $N = 94$ , where the lowest energy configuration is  $D_2$ , while two additional configurations with other symmetries,  $C_s$  and  $C_3$ , with total Coulomb energies only higher in the fifth significant figure were found. All three configurations are shown in Figure 8.

While experience both in the present investigation and elsewhere leads us to associate symmetry with low energy, there is as far as we are aware, no general theorem to this effect. In fact we may note that three of the minimal energy configurations we list have no overall symmetry apparent. In each of the cases we have found a symmetric configuration with total configuration energy higher than the non-symmetric case only in the sixth significant figure. The total Coulomb energy for each configuration is listed in the tables in the Appendix and also in Table 2.

### 3.2 Isoenergy Subsets

An interesting feature can be observed from inspection of the tables of coordinates and individual particle energies of the equilibrium configurations given in the Appendix. It is seen there that the points break down into equal point energy (isoenergy) subsets. Clearly, if two points of a configuration can be transformed into one another by an operation of the symmetry group of the configuration, then those two points are equivalent. In a very few cases (e.g.,  $N = 12$ , see reference 1), all points are equivalent and in that case have equal particle energies. Inspection of a few of the tables however reveals that for most configurations, the points separate into isoenergy subsets of two or more equivalent points. For the points of a subset to be equivalent, the subset must have at least as high a symmetry group as the total configuration. (Of course when there are two or more different interactions as between atoms within molecules and between molecules, there may be local symmetries within the molecules, which are lower order than the overall symmetry.) An isoenergy subset may consist of just one point, only when the point is located on a rotation axis or reflection plane. Numerous two point isoenergy subgroups occur for configurations with  $C_s$  or  $C_2$  symmetry groups.



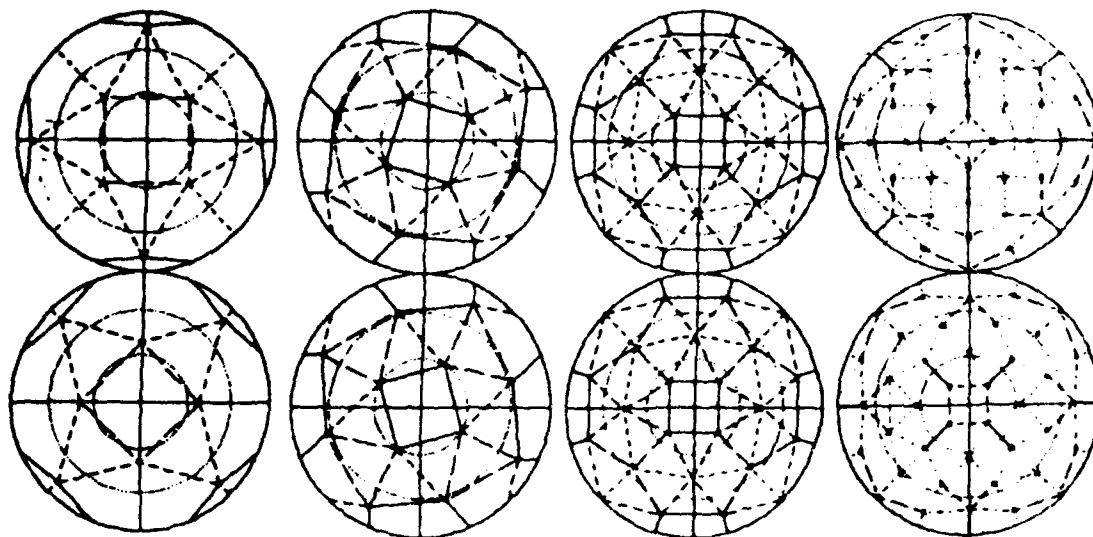


Figure 6. Figures with four-fold rotational symmetry showing self-similarity as  $N$  increases. From the left,  $N = 16$ ;  $N = 24$ ;  $N = 44$ ;  $N = 80$ . The  $N = 16$  figure is not the minimal energy configuration, the others are.

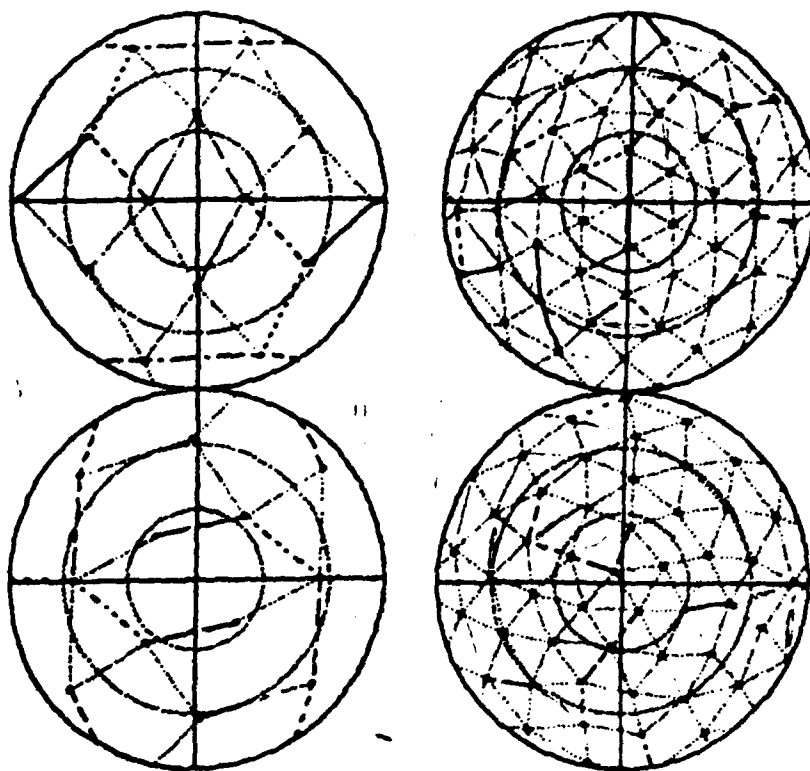


Figure 7. Figures for  $N = 26$  (on the left) and  $N = 99$ , arranged to show an approximate bilateral symmetry which occurs in one hemisphere only.

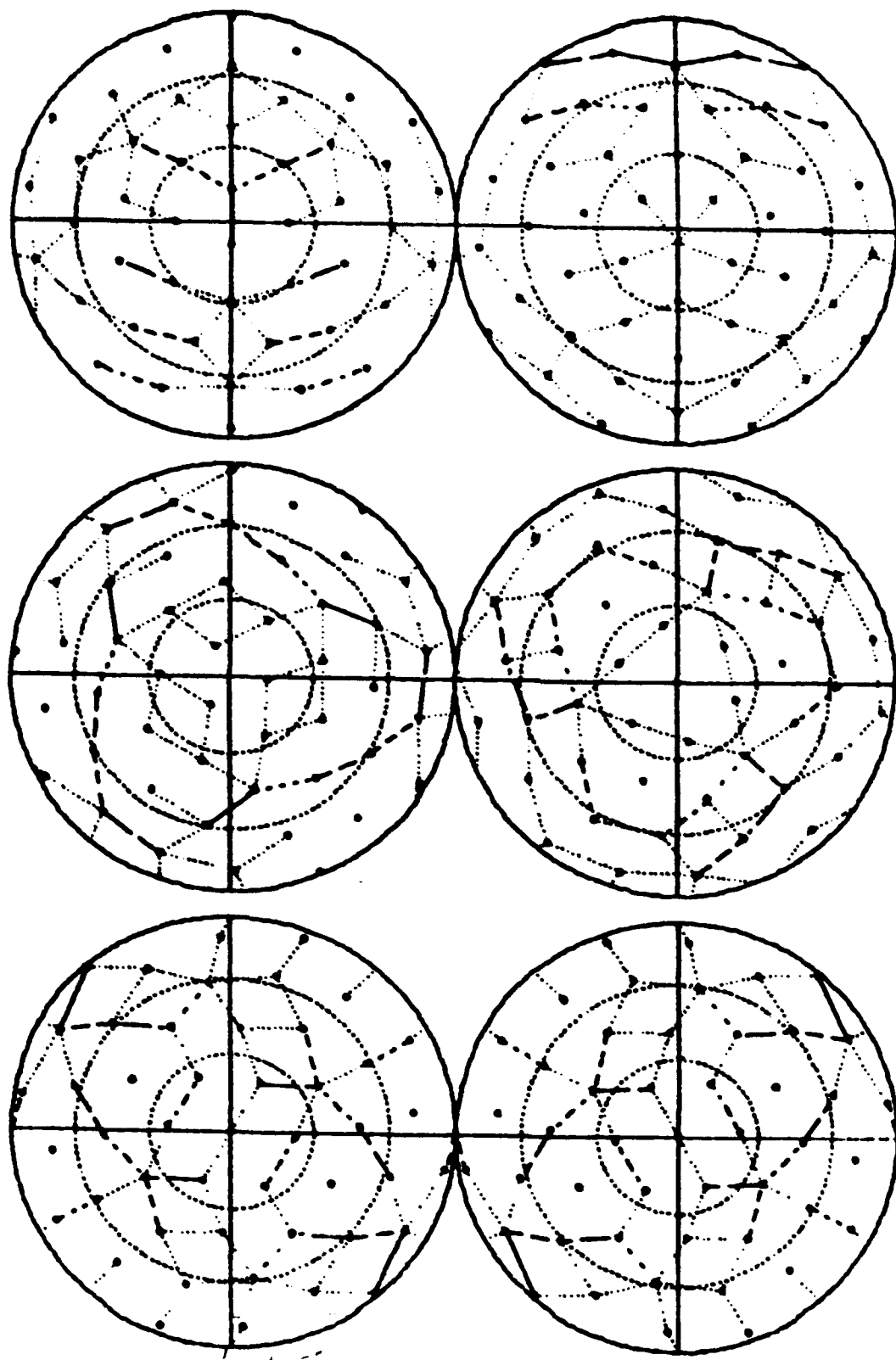


Figure 8. The "three faces of  $N = 94$ ". From the left, the symmetries are  $D_2$  (minimal energy),  $C_3$ , and  $C_s$ . Coulomb energies of all three figures agree to four significant figures.

When the configuration is characterized by a high symmetry group the above rule can lead to an interlacing of symmetric polyhedra. Consider for example the configuration for 44 charged points which is octahedral, with all possible reflection planes. (See Figure 9.) Its points are divided into three equal energy subsets: There are 8 points in the subset with the highest point energies (call this subset 1). Subset 2, with the next higher point energies has 12 points, and subset 3 has 24.

The subset geometries all have octahedral symmetry. Subset 2 consists of a cuboctahedron (i.e., an octahedron with truncating planes normal to the long axes with the squares at the intersections of the planes and octahedron just large enough to meet the four neighboring squares corner to corner.) The eight points of subset 1 form a cube with corners above the centers of the eight equilateral triangles formed between the squares of the octahedron of subset 2. Subset 3 consists of six squares above the centers of the truncating squares of subset 2 but rotated by 45 degrees so their neighboring sides are parallel. The dissection of the 44 point equilibrium figure is shown in Figure 9.

The 72 point icosahedral figure (see Figure 3) consists of two sets: a twelve point icosahedron equal energy set and a sixty point set of slightly lower point energies, consisting of twelve equilateral pentagons. Each pentagon surrounds the vertices of the forgoing icosahedron with each point 24.492 degrees along a great circle from the corresponding vertex.

The 48 point configuration has octahedral symmetry. The individual points separate into two isoenergy subsets of twenty-four points each. The higher energy of these consists of six squares normal to the diameter at the corners of an octahedron, with the squares which are on opposite ends of the sphere's diameter twisted by 37.26 degrees with respect to one another. The other set of 24 points consists of eight equivalent equilateral triangles placed above the middle of the triangular faces of the "octahedron" of the first set. If one joins the midpoints of two equilateral triangles on opposite ends of a diameter, one has a three-fold symmetry axis corresponding to joining the midpoints of opposite faces of the "snubbed octahedron" of the 24 point higher energy set. This dissection of the 48 point figure is shown in Figure 10.

It is possible for an isoenergy subset to have higher symmetry than the whole set. There are numerous examples with one or two points at the poles (e.g.,  $n$  equal to 83 or 84) for which all the other points have some rotational symmetry about the axis between the poles. Then the subset consisting of the pole points considered by themselves has symmetry  $C_{\infty}$ .

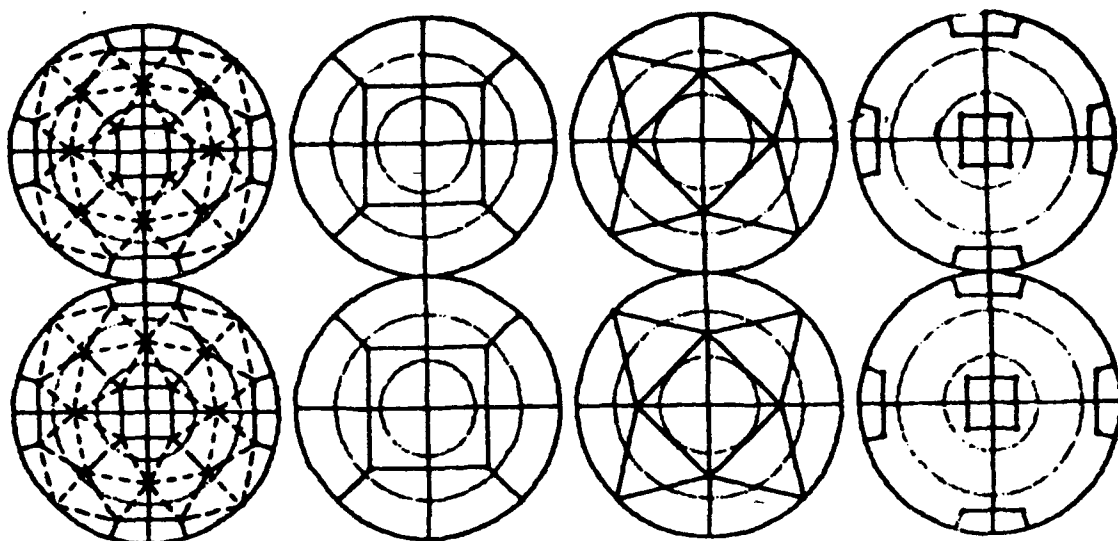


Figure 9. The equilibrium figure for  $N = 44$  with its isoenergy subsets shown to the right. From left to right, the cube has highest individual particle energies, the cuboctahedron is next and the truncated octahedron has lowest individual particle energies.

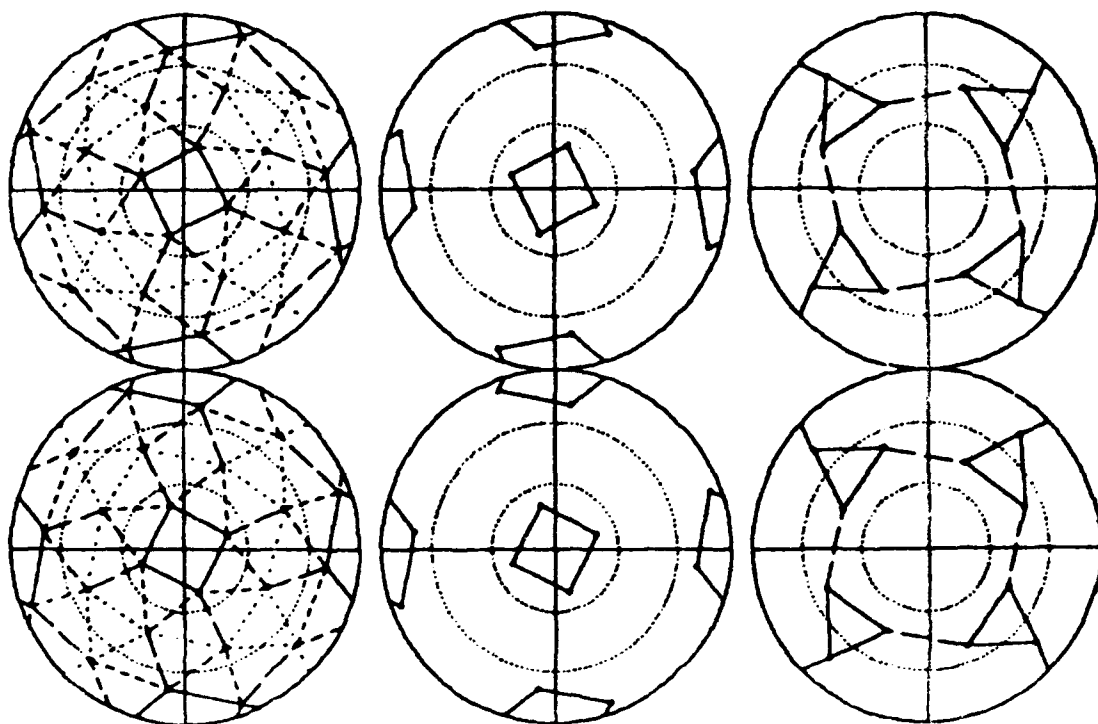


Figure 10. The equilibrium figure for  $N = 48$  with its two isoenergy subsets shown to the right. The lower individual particle energies belong to the subset with its points arranged in eight triangles.

A less trivial example for which an isoenergy subset has higher symmetry than the whole set of points is the configuration for 46 charged points. The total set has tetrahedral symmetry, but inspection of its table of points indicates a six point isoenergy subset with octahedral symmetry. This consists of the three points with theta equal to  $\sim 54.7$  degrees and three with theta  $\sim 125.26$  degrees. These points bisect the edges of the spherical tetrahedron formed by the four point isoenergy subset. Besides these two subsets there are three additional isoenergy subsets of twelve points each. Each twelve point isoenergy subset is divided into four sets of three points. Those three points are related to each other by the three-fold symmetric rotation subgroup at each corner of the tetrahedron.

### 3.3 Configuration Energies

The total coulomb energy of each configuration is just one half the sum of the individual particle energies and is listed with each configuration in the Appendix. It is of interest to obtain an approximation for this value based on general features of point charges spread evenly over the surface of a sphere.

To obtain the first approximation, we spread charge 1 uniformly over the surface of the sphere. The energy to bring up charge 2 is then  $u_2 = q^2/(4\pi\epsilon_0 R)$ , where  $R$  is the radius of the sphere and  $q$  is the charge per point charge. Similarly, the energy to bring up the third charge is  $u_3 = 2q^2/(4\pi\epsilon_0 R)$ , and so on giving for the first approximation to the total Coulomb energy, the sum of these terms or

$$U_1 = [N(N-1)/2](q^2/(4\pi\epsilon_0 R))$$

where  $N$  is the total number of point charges on the sphere. While the above gives a reasonable value, the approximation may be improved by accounting for the bare area around each point charge on the surface. Setting the area around a charge at the pole of the sphere equal to the average area per charge on the sphere gives

$$2\pi \int_0^{\theta_N} [R^2 \sin(\theta) d\theta] = 4\pi R^2/N$$

Integrating, and expanding in theta we find

$$\Theta_N = 2/N^{1/2}$$

The interaction energy which is to be subtracted is then

$$U_2 = 2\pi \int_0^{\Theta_N} (\Phi * \Sigma \sin \theta) d\theta$$

where  $\Phi$  is the potential due to the point charge at the center of the bare area and is approximately equal to  $q/4\pi\epsilon_0 R \sin \theta$  and  $\Sigma$  is the surface charge per unit area on the sphere and is  $(N-1)q/4\pi R^2$ . Substituting this into the above equation gives

$$U_2 = (N - 1)q/RN^{1/2}$$

Now  $U_2$  is for one interaction, hence for all such interactions we must multiply by  $N$  and divide by 2, since each charge is counted twice, once as a point charge and once smeared out. Subtracting  $N*U_2/2$  from  $U_1$  then gives for the total coulomb energy

$$U_{app} = [N(N - 1)q^2/(4\pi\epsilon_0 R)][1 - 1/N^{1/2}]/2$$

The numerical values listed are calculated with  $R = q = 1/4\pi\epsilon_0 = 1$ . In Table 2, the first column gives the number of charges on the sphere, the second column is the exact total coulomb energy,  $U_T$ , the third is the approximate value,  $U_{app}$ , and the fourth,  $\Delta$ , is the difference between the fourth and third columns, giving the error in the approximation. A plot of  $\Delta$  vs charge number is given in Figure 11 showing a roughly parabolic dependence on  $N$ . The error of the approximation is very small ( $< .3\%$  for all cases considered) but is growing at the same rate as the total Coulomb energy and thus is expected to approach a constant percentage of the total value.

TABLE 2  
Summary of Energy Information

N	U <sub>T</sub>	U <sub>app</sub>	del	eVar	Edge Def.
3	1.73205	1.26795	-0.46410	zero	0
4	3.67423	3.00000	-0.67423	zero	0
5	6.47469	5.52786	-0.94683	2.02e-2	0
6	9.98528	8.87628	-1.10900	zero	0
7	14.4530	13.0627	-1.39023	3.18e-2	0
8	19.6753	18.1005	-1.57478	zero	2
9	25.7600	24.0000	-1.75999	8.91e-3	0
10	32.7169	30.7698	-1.94720	9.64e-3	0
11	40.5965	38.4169	-2.17957	1.90e-2	0
12	49.1652	46.9474	-2.21781	zero	0
13	58.8532	56.3667	-2.48653	1.98e-2	0
14	69.3064	66.6792	-2.62713	1.59e-2	0
15	80.6702	77.8891	-2.78112	1.13e-2	0
16	92.9117	90.0000	-2.91165	1.03e-2	0
17	106.050	103.015	-3.03525	5.95e-4	0
18	120.084	116.938	-3.14690	5.37e-3	0
19	135.089	131.770	-3.31955	1.05e-2	1
20	150.882	147.515	-3.36685	4.13e-3	0
21	167.642	164.174	-3.46736	6.96e-3	0
22	185.288	181.751	-3.53690	3.13e-3	0
23	203.930	200.246	-3.68433	8.31e-3	0
24	223.347	219.662	-3.68535	zero	6
25	243.813	240.000	-3.81276	8.63e-3	1
26	265.133	261.262	-3.87109	9.42e-3	0
27	287.303	283.450	-3.85260	3.12e-3	0
28	310.492	306.565	-3.92685	4.40e-3	0
29	334.634	330.608	-4.02673	7.17e-3	0
30	359.604	355.580	-4.02371	4.51e-3	0
31	385.531	381.484	-4.04730	6.77e-3	0
32	412.261	408.319	-3.94250	2.23e-3	0
33	440.204	436.087	-4.11707	9.27e-3	2
34	468.905	464.789	-4.11557	6.13e-3	0
35	498.570	494.427	-4.14325	6.88e-3	0
36	529.122	525.000	-4.12244	5.15e-3	0
37	560.628	556.510	-4.11768	6.82e-3	0
38	593.049	588.958	-4.09064	6.45e-3	0
39	626.389	622.345	-4.04401	4.53e-3	0
40	660.725	656.671	-4.05414	4.43e-3	0
41	695.917	691.938	3.97925	5.58e-3	0
42	732.078	728.145	-3.93335	4.35e-3	0
43	769.191	765.294	-3.89703	5.23e-3	0
44	807.174	803.385	-3.78912	2.80e-3	6
45	846.188	842.419	-3.76892	3.26e-3	0
46	886.167	882.398	-3.76953	3.84e-3	0
47	927.062	923.320	-3.74231	6.13e-3	1
48	968.713	965.187	-3.52618	1.96e-3	6
49	1011.56	1008.00	-3.55719	4.45e-3	0
50	1055.18	1051.76	-3.42346	4.08e-3	0
51	1099.82	1096.46	-3.35498	3.59e-3	0
52	1145.42	1142.12	-3.30200	4.61e-3	-
53	1191.92	1188.72	-3.20508	5.50e-3	-
54	1239.36	1236.27	-3.09595	4.03e-3	-
55	1287.77	1284.76	-3.01001	5.02e-3	-
56	1337.10	1334.21	-2.88647	3.70e-3	-

TABLE 2  
(Continued)

N	U <sub>T</sub>	U <sub>app</sub>	del	eVar	Edge Def.
57	1387.38	1384.60	-2.77844	3.70e-3	-
58	1438.62	1435.95	-2.66772	5.04e-3	-
59	1490.77	1488.25	-2.52649	4.81e-3	-
60	1543.83	1541.49	-2.33643	3.29e-3	-
61	1597.94	1595.69	-2.24927	-	-
62	1652.93	1650.84	-2.08582	-	-
63	1708.88	1706.95	-1.93445	-	-
64	1765.80	1764.00	-1.80261	-	-
65	1823.67	1822.01	-1.66016	-	-
66	1882.44	1880.97	-1.47266	-	-
67	1942.12	1940.88	-1.23926	-	-
68	2002.87	2001.75	-1.12280	-	-
69	2064.54	2063.57	-0.961182	-	-
70	2127.13	2126.35	-0.774414	-	-
71	2190.65	2190.08	-0.565186	-	-
72	2255.00	2254.77	-0.228760	-	-
73	2320.63	2320.42	-0.218018	-	-
74	2387.09	2387.02	-7.22656e-02	-	-
75	2454.37	2454.57	0.200928	-	-
76	2522.67	2523.08	0.407715	-	0
77	2591.85	2592.55	0.701172	-	0
78	2662.05	2662.98	0.929932	-	0
79	2733.25	2734.36	1.11206	-	1
80	2805.36	2806.70	1.34521	-	2
81	2878.52	2880.00	1.47705	-	0
82	2952.57	2954.26	1.68237	-	0
83	3027.53	3029.47	1.94360	-	0
84	3103.47	3105.65	2.18115	-	0
85	3180.39	3182.78	2.38989	-	0
86	3258.22	3260.87	2.65112	-	0
87	3337.00	3339.92	2.92212	3.81e-3	0
88	3416.73	3419.93	3.20093	3.83e-3	0
89	3497.44	3500.91	3.46606	4.19e-3	0
90	3579.18	3582.84	3.65918	3.83e-3	0
91	3661.71	3665.73	4.01367	4.01e-3	0
92	3745.34	3749.58	4.24072	4.06e-3	0
93	3829.84	3834.39	4.54785	4.25e-3	0
94	3915.31	3920.17	4.85645	3.93e-3	0
95	4001.77	4006.90	5.12891	3.94e-3	0
96	4089.15	4094.60	5.44312	3.04e-3	0
97	4177.53	4183.25	5.72119	3.87e-3	0
98	4266.82	4272.87	6.05225	3.44e-3	0
99	4357.14	4363.46	6.31689	3.80e-3	0
100	4448.35	4455.00	6.64893	3.14e-3	0
101	4540.59	4547.51	6.91650	3.36e-3	0
102	4633.74	4640.98	7.23877	2.98e-3	0
103	4727.84	4735.41	7.57031	3.30e-3	0
104	4822.93	4830.80	7.87451	3.35e-3	0
105	4919.06	4927.16	8.10205	3.74e-3	0
106	5015.98	5024.48	8.49512	3.15e-3	0
107	5113.98	5122.76	8.78271	-	-
108	5212.81	5222.01	9.19824	-	-
250	29068.2	29156.5	88.3301	-	-



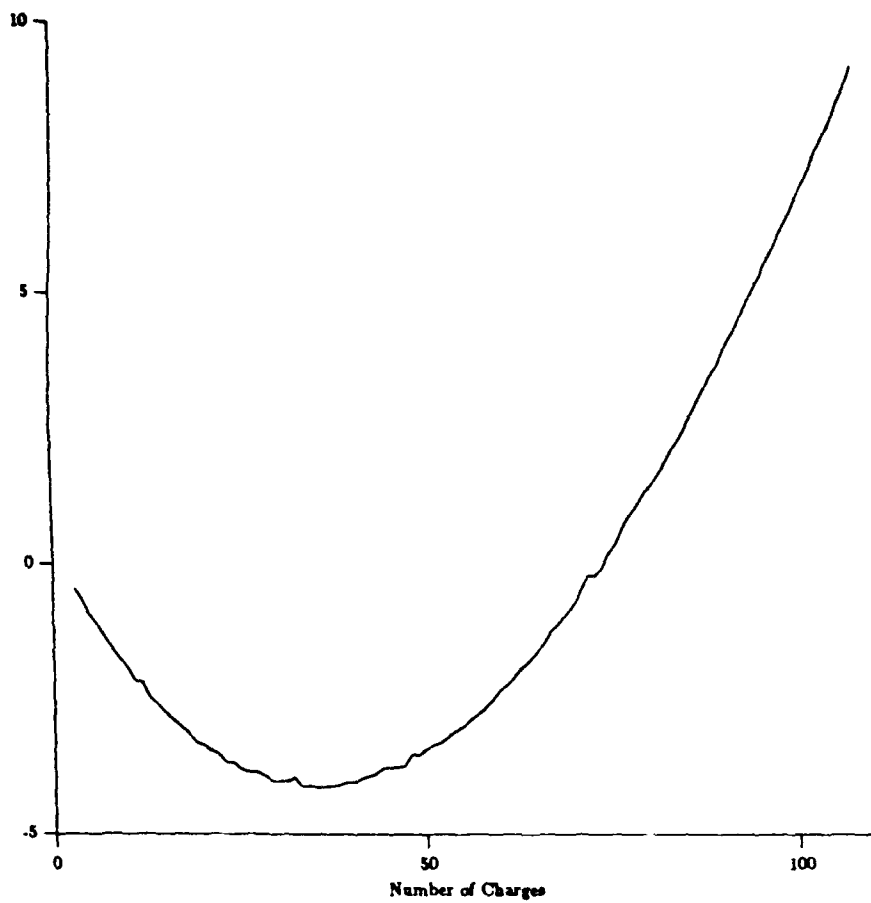


Figure 11. The difference between  $U_{app}$  and  $U_T$  is plotted against total number of charges and is approximately parabolic in form.

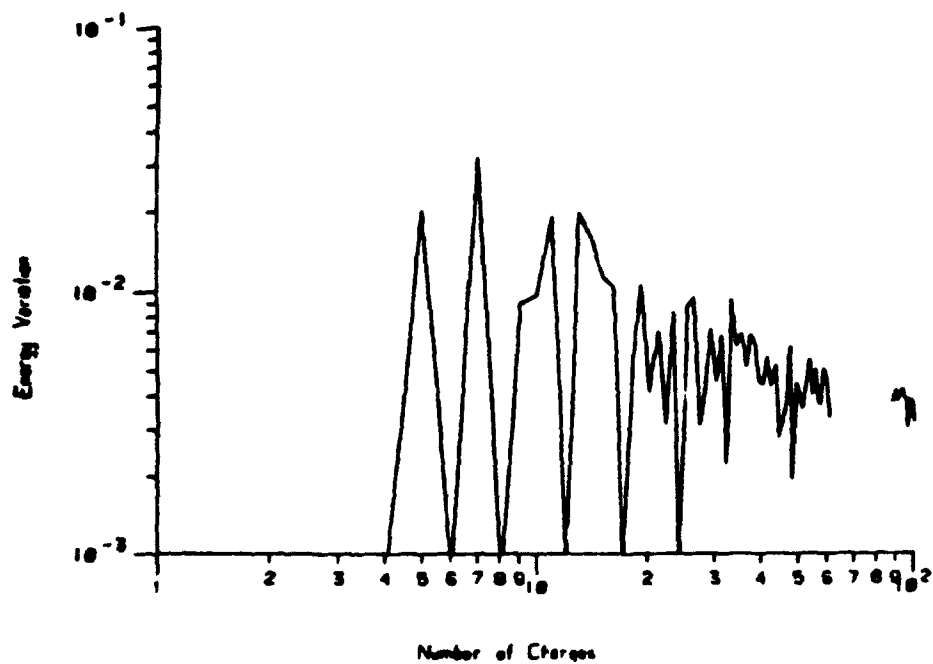


Figure 12. A logarithmic plot of the relative single particle energy variation (eVar) vs charge number  $N$ .

### 3.4 Dependence of Individual Particle Energy on Total Charge Number

It would seem that the minimal energy configuration is reached when the individual particles (charges) are as much like one another as the geometrical constraints allow. This may be quantitated by defining the variability in the single particle energies for a given charge number as the difference between the highest and the lowest single particle energies divided by the average of these quantities. This is listed in the fifth column as Table 2 as  $eVar$ , which is plotted against charge number on a log-log plot in Figure 12. There are zero values early on, however the slope of the envelope of points suggests that  $eVar$ , the single particle variability as a fraction of the average single particle energy, approaches zero as fast or faster than  $N^{-1/2}$ .

### 3.5 Configuration of the Polyhedron between Charges

For a given charge number we may define an empirical polyhedron for the minimum equilibrium energy as follows: Connect neighboring charges on the sphere with straight lines proceeding from the shortest to longer in order, until the first crossing of these lines. The number of connecting lines before such a crossing occurs is then defined to be the number of edges of the empirical polyhedron. Multiplying this number by two and dividing by the charge number gives an average number of edge neighbors. It is interesting to define an quantity called the "Edge Defect" in the following manner.

$$\text{Edge Defect} = [3N - \text{Number of Edges} - 6]$$

We have constructed the empirical polyhedron for most of the examples studied and listed the Edge Defect for those polyhedra in Table 2. It is straight-forward to show (e.g., by induction) that for any closed polyhedron consisting entirely of triangular faces that the Edge Defect is identically zero. Hence when the Edge Defect  $> 0$ , (it can't be less) either the polyhedron has plane nontriangular faces or there is a polygon for which a crossing occurs before the polyhedron is complete. (In the case of nontriangular plane faces, it is easy to see that by continuing to connect vertices across plane polygonal faces, one again arrives at a triangular polyhedron and a zero value for the Edge Defect.) It is seen in Table 2 that the departures from zero for the values of the Edge Defect are sparse, and do not increase with  $N$ . From this and the above equation, we deduce that the number of "edge neighbors" for each vertex in the empirical polyhedron approaches six as  $N$  becomes large. Each case with the Edge Defect unequal to

zero was examined. In every case except  $N = 33$ , the crossing occurred across a quadrilateral face which completed the empirical polyhedron, so that the quadrilateral face has two equal diagonals which are shorter than any other sides of the polyhedron. In the one exceptional case found, a quadrilateral with equal diagonals occurred on the step before a non-planar quadrilateral was separated into two triangles by an edge. The symmetry group for  $N=33$  is  $C_s$  and the two quadrilaterals mentioned are bisected by the single symmetry plane. In all other cases found, the plane quadrilateral either spanned a  $C_s$  symmetry plane or was perpendicular to an axis of four-fold rotational symmetry. This occurred with the  $C_s$  symmetry sequentially with charge number either before or after the four-fold symmetry in three separate instances.

From the above equation relating vertices and edges for a polyhedron made up of all triangular faces, one may obtain an interesting numerical relationship. Let the number of vertices having four edges each be  $m$ , the number with five edges be  $p$ , and the number with seven edges be  $q$ . Then

$$2m + p - q = 12$$

The same relationship may also be obtained from the spherical excess of  $4\pi$  over the total number of radians making up the triangles dividing up a sphere. If there were a seven-edged regular polygon as a face of the polyhedron, then by adding one point at the center of the polygon, one obtains a seven-edged vertex. Then the above equation indicates that several four and/or five-edged vertices would already be present. Hence the charges would be unevenly spread over the face of the sphere. Similarly a seven-edged vertex would require four and/or five-edged vertices. Since the lowest energy configuration tends to make the individual particle energies and thus their local environments more alike, the nonuniformity caused by a seven-edged vertex makes seven-fold symmetry unlikely.

### 3.6 Quasicontinuity of the Configurations

In reference 2, we pointed out that one may see geometries which are almost continuous, at least on one face as one changes the charge number from  $N$  to  $N + 1$ . As the charge number becomes larger, this quasicontinuity is quite apparent if the two configurations are examined carefully and properly superposed. This is illustrated for the two sequences: 47, 48, 49 and 99, 100, 101 in Figures 13 and 14. In each case, the closeness of the geometries for succeeding  $N$  values is apparent although the symmetries change sharply from  $C_s$  to octahedral to  $C_3$  in the first case, and from  $D_2$  to tetrahedral to  $C_3$

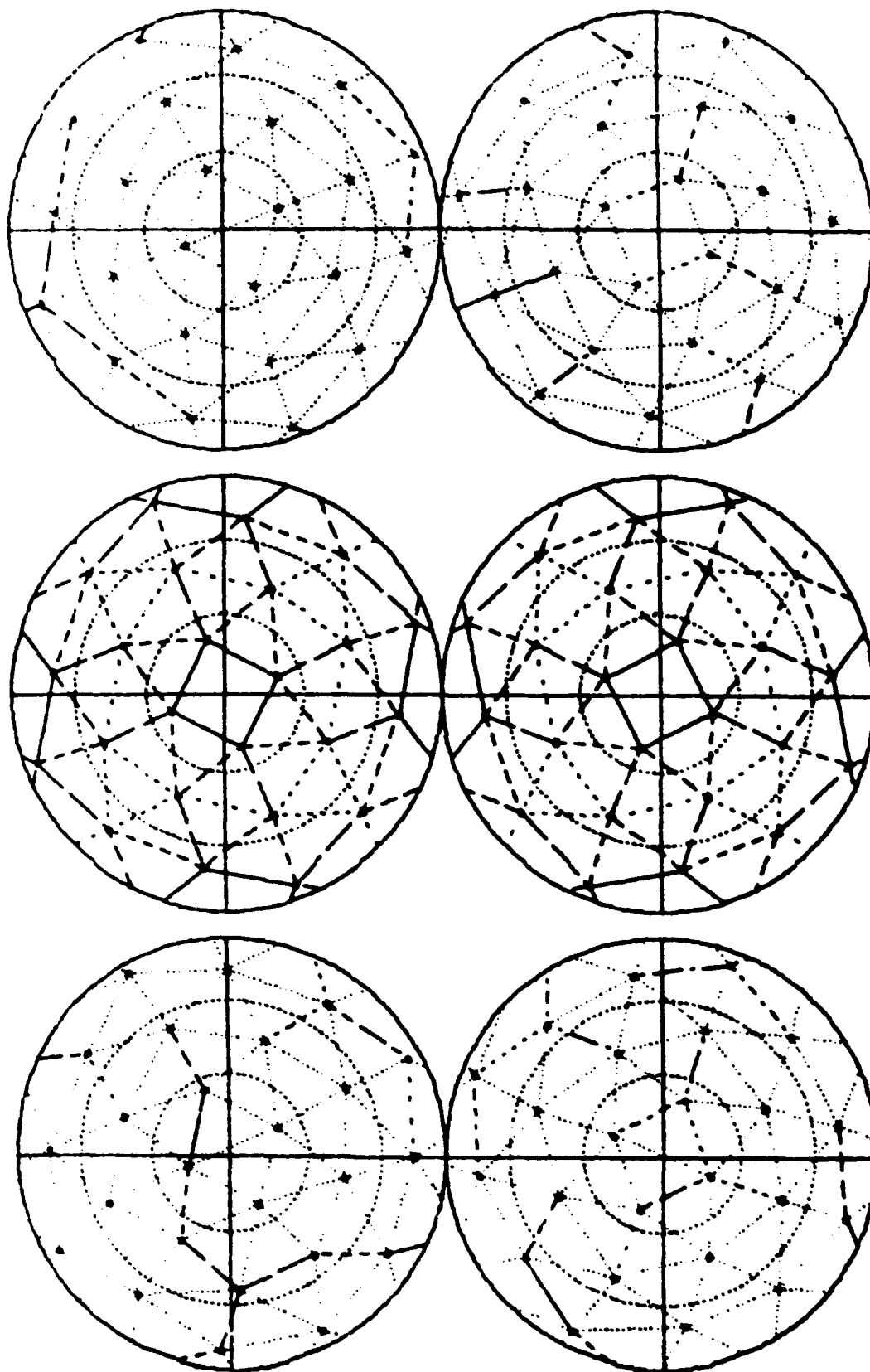


Figure 13. The equilibrium figures for (left to right)  $N = 47$ ,  $N = 48$ , and  $N = 49$  are shown in orientations selected to show that the figures change by very small decrements as  $N$  increases by one.

in the second. The equilibrium figures are aligned to show their similarity rather than their symmetry group, but this may be displayed by plotting the figures in the orientation given in the tables of the Appendix. In Figure 15, the equilibrium figures for  $N = 99$  is superposed over that for  $N = 100$ . A similar superposition is shown for  $N = 100$  and  $101$ . Inspection of the figures shows that succeeding  $N$  values give rise to many corresponding points which are very close on the sphere. In each of the superpositions, there is one hemisphere for which most of the points are close to coincidence. This feature appears to be a requirement which succeeding  $N$  values satisfy in many cases.

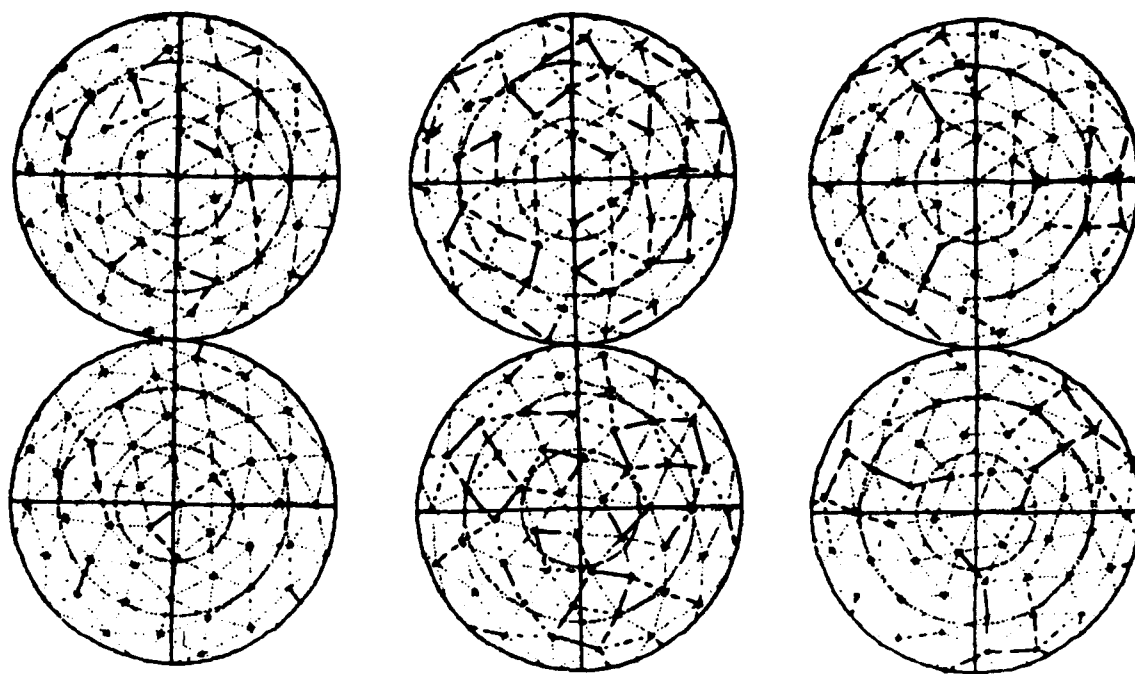


Figure 14. The equilibrium figures for (left to right)  $N = 99$ ;  $N = 100$ ;  $N = 101$  oriented so as to show similarity of consecutive figures.

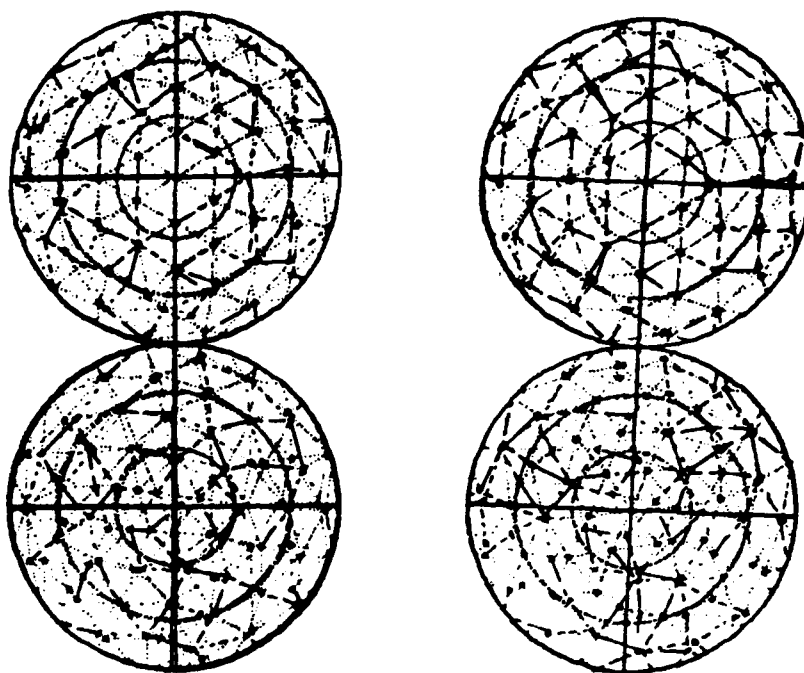


Figure 15. The graphs of Figure 14 superposed. On the left, 99/100; on the right, 100/101.

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**APPENDIX**  
**Tables of Coordinates**

**34 POINTS**  
**D<sub>2</sub>**

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
6	40.941839	148.337730	.27490157+02	2	35.772562	27.759775	.27600401+02
7	40.941839	-31.662267	.27490157+02	3	35.772563	-152.240227	.27600401+02
28	139.058159	-148.337730	.27490157+02	32	144.227434	152.240223	.27600400+02
29	139.058159	31.662267	.27490157+02	33	144.227434	-27.759773	.27600401+02
1	.000000	.000000	.27512290+02	8	68.965414	45.956758	.27626308+02
34	179.999998	-38.197842	.27512289+02	9	68.965414	-134.043242	.27626308+02
4	38.451528	89.699944	.27513373+02	26	111.034585	134.043240	.27626308+02
5	38.451528	-90.300054	.27513373+02	27	111.034585	-45.956758	.27626308+02
30	141.548470	90.300055	.27513373+02	16	79.544349	152.559719	.27640788+02
31	141.548470	-89.699944	.27513373+02	17	79.544349	-27.440277	.27640789+02
12	70.722882	117.834849	.27575102+02	18	100.455649	-152.559721	.27640788+02
13	70.722882	-62.165149	.27575102+02	19	100.455650	27.440277	.27640789+02
22	109.277116	62.165148	.27575102+02	14	74.526101	-99.427771	.27659280+02
23	109.277116	-117.834851	.27575102+02	15	74.526101	80.572227	.27659280+02
10	69.126155	6.165333	.27590873+02	20	105.473896	99.427770	.27659280+02
11	69.126156	-173.834665	.27590872+02	21	105.473896	-80.572227	.27659280+02
24	110.873843	173.834665	.27590872+02				
25	110.873843	-6.165333	.27590873+02				

Total Coulomb Energy: 468.90485328

**35 POINTS**  
**C<sub>2</sub>**

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
22	104.661765	91.413797	.28400846+02	26	114.222973	161.402802	.28482390+02
23	104.661765	-88.586203	.28400846+02	27	114.222973	-18.597198	.28482390+02
32	146.186302	-177.016277	.28421656+02	16	83.138281	179.524761	.28485637+02
33	146.186302	2.983721	.28421656+02	17	83.138281	-.475239	.28485637+02
6	41.583106	.000000	.28426941+02	4	35.979967	57.088655	.28504847+02
7	41.583106	180.000000	.28426941+02	5	35.979967	-122.911346	.28504847+02
30	132.251345	61.868395	.28449512+02	8	67.399415	-31.692247	.28512125+02
31	132.251345	-118.131605	.28449512+02	9	67.399416	148.307753	.28512125+02
1	.000000	.000000	.28450160+02	10	68.329546	72.675108	.28550207+02
24	112.165929	21.713769	.28455337+02	11	68.329546	-107.324892	.28550207+02
25	112.165929	-158.286230	.28455337+02	18	97.681881	-125.752694	.28552867+02
12	69.046407	31.722194	.28455478+02	19	97.681882	54.247306	.28552867+02
13	69.046407	-148.277805	.28455478+02	20	97.815422	129.731916	.28553939+02
28	132.041319	120.371936	.28465035+02	21	97.815422	-50.268083	.28553939+02
29	132.041319	-59.628064	.28465035+02	14	69.973118	108.126673	.28555189+02
2	35.979399	120.441429	.28475968+02	15	69.973118	-71.873327	.28555189+02
3	35.979399	-59.558571	.28475968+02	34	162.960932	93.431048	.28596819+02
				35	162.960932	-86.568952	.28596819+02

Total Coulomb Energy: 498.56987249

## 37 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
26	113.053318	1.300848	.30203259+02	16	78.495763	11.924308	.30309022+02
27	113.053322	-178.699146	.30203258+02	17	78.495766	-168.075687	.30309021+02
6	39.915896	-161.348396	.30226027+02	14	69.611712	87.490030	.30320912+02
7	39.915897	18.651599	.30226028+02	15	69.611714	-92.509968	.30320912+02
12	67.408350	-131.291817	.30238311+02	34	147.953018	.000000	.30331428+02
13	67.408351	48.708182	.30238311+02	35	147.953020	-179.999996	.30331427+02
18	94.955276	150.392681	.30239670+02	32	132.523172	47.662875	.30331812+02
19	94.955276	-29.607318	.30239671+02	33	132.523172	-132.337120	.30331812+02
20	98.593668	112.461268	.30271366+02	10	66.605442	-56.374146	.30352427+02
21	98.593668	-67.538728	.30271366+02	11	66.605443	123.625855	.30352426+02
28	127.451754	-41.485940	.30274994+02	24	100.994858	36.934725	.30363848+02
29	127.451756	138.514055	.30274993+02	25	100.994858	-143.065269	.30363848+02
22	99.444108	72.240180	.30278822+02	30	128.142454	93.778753	.30366250+02
23	99.444110	-107.759816	.30278822+02	31	128.142454	-86.221242	.30366250+02
1	.000000	.000000	.30286096+02	2	33.458584	-43.662714	.30372179+02
4	36.902015	75.405645	.30295172+02	3	33.458585	136.337280	.30372178+02
5	36.902017	-104.594350	.30295172+02	8	63.023404	-17.888873	.30409922+02
36	162.298685	95.244849	.30299507+02	9	63.023404	162.111128	.30409921+02
37	162.298685	-84.755138	.30299507+02				

Total Coulomb Energy: 560.62797306

## 38 POINTS

C<sub>2v</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
37	162.958105	-90.000002	.31126740+02	29	123.480221	90.000000	.31231635+02
38	162.958107	90.000000	.31126740+02	30	123.480221	-90.000000	.31231635+02
25	110.228068	162.147556	.31150491+02	21	100.742132	121.072636	.31244959+02
26	110.228069	-162.147556	.31150491+02	22	100.742132	-121.072636	.31244959+02
27	110.228071	17.852441	.31150492+02	23	100.742133	58.927361	.31244960+02
28	110.228071	-17.852441	.31150492+02	24	100.742133	-58.927361	.31244960+02
3	31.672109	90.000000	.31152571+02	19	87.048971	-90.000000	.31252133+02
4	31.672110	-89.999998	.31152571+02	20	87.048972	89.999998	.31252133+02
13	76.647893	179.999998	.31156641+02	31	133.590315	48.390510	.31276119+02
14	76.647895	.000000	.31156641+02	32	133.590315	131.609489	.31276119+02
9	61.324022	113.042035	.31158339+02	33	133.590315	-131.609488	.31276119+02
10	61.324023	66.957959	.31158339+02	34	133.590317	-48.390511	.31276119+02
11	61.324023	-113.042036	.31158339+02	15	79.703662	145.689293	.31288698+02
12	61.324024	-66.957961	.31158339+02	16	79.703663	-145.689295	.31288698+02
35	145.938150	-.000001	.31187399+02	17	79.703664	34.310704	.31288699+02
36	145.938150	-179.999996	.31187399+02	18	79.703665	-34.310704	.31288699+02
5	46.807281	26.247715	.31188302+02	1	16.456362	-179.999998	.31328004+02
6	46.807281	153.752281	.31188302+02	2	16.456364	-.000005	.31328005+02
7	46.807281	-153.752281	.31188302+02				
8	46.807281	-26.247717	.31188302+02				

Total Coulomb Energy: 593.04894354

## 39 POINTS

 $D_{3vh}$ 

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
7	57.277985	19.677820	.32054996+02	13	71.143928	179.999998	.32166957+02
8	57.277985	100.322178	.32054996+02	14	71.143929	60.000000	.32166957+02
9	57.277986	139.677820	.32054996+02	15	71.143930	-60.000000	.32166957+02
10	57.277986	-139.677820	.32054995+02	25	108.856069	60.000000	.32166957+02
11	57.277986	-100.322178	.32054996+02	26	108.856069	-179.999998	.32166956+02
12	57.277986	-19.677821	.32054996+02	27	108.856070	-60.000000	.32166957+02
28	122.722011	139.677818	.32054995+02	16	89.999998	-152.052948	.32198849+02
29	122.722012	100.322179	.32054995+02	17	89.999998	-32.052950	.32198849+02
30	122.722013	19.677820	.32054995+02	19	89.999999	87.947049	.32198849+02
31	122.722013	-139.677820	.32054995+02	21	89.999999	152.052948	.32198849+02
32	122.722013	-100.322179	.32054995+02	23	90.000000	32.052948	.32198849+02
33	122.722015	-19.677821	.32054995+02	24	90.000000	-87.947049	.32198849+02
1	21.516623	119.999997	.32066237+02	4	38.942417	59.999998	.32200432+02
2	21.516624	.000001	.32066237+02	5	38.942417	179.999998	.32200432+02
3	21.516624	-119.999997	.32066237+02	6	38.942418	-59.999999	.32200432+02
37	158.483376	.000000	.32066237+02	34	141.057581	60.000000	.32200432+02
38	158.483376	119.999999	.32066237+02	35	141.057581	-179.999998	.32200431+02
39	158.483376	-119.999999	.32066237+02	36	141.057581	-60.000000	.32200432+02
18	89.999999	.000000	.32107742+02	Total Coulomb Energy: 626.38900902			
20	89.999999	119.999997	.32107742+02				
22	89.999999	-119.999999	.32107742+02				

## 40 POINTS

 $D_2$ 

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
13	72.294863	7.222406	.32958815+02	15	73.168655	85.076248	.33041894+02
14	72.294864	-172.777594	.32958813+02	16	73.168659	-94.923749	.33041894+02
27	107.705178	-7.222406	.32958814+02	25	106.831285	94.923739	.33041894+02
28	107.705181	172.777590	.32958813+02	26	106.831286	-85.076257	.33041894+02
1	16.172861	125.281963	.32971157+02	9	52.675376	118.149953	.33075778+02
2	16.172862	-54.718042	.32971157+02	10	52.675377	-61.850045	.33075778+02
39	163.827126	54.718160	.32971155+02	31	127.324586	61.850031	.33075777+02
40	163.827133	-125.281838	.32971154+02	32	127.324588	-118.149965	.33075777+02
11	65.656073	43.311718	.32977698+02	19	85.187549	119.522346	.33077232+02
12	65.656075	-136.688278	.32977697+02	20	85.187550	-60.477650	.33077232+02
29	114.343923	136.688253	.32977697+02	21	94.812413	60.477655	.33077233+02
30	114.343924	-43.311738	.32977697+02	22	94.812417	-119.522342	.33077232+02
17	81.613484	-27.537003	.33024192+02	5	41.523134	74.252752	.33103826+02
18	81.613484	152.462992	.33024191+02	6	41.523138	-105.747246	.33103826+02
23	98.386551	27.537011	.33024191+02	35	138.476805	105.747195	.33103825+02
24	98.386554	-152.462984	.33024190+02	36	138.476809	-74.252797	.33103825+02
3	34.642294	22.477751	.33027009+02	7	49.088027	-21.019617	.33105058+02
4	34.642297	-157.522242	.33027008+02	8	49.088027	158.980381	.33105057+02
37	145.357735	-22.477821	.33027007+02	33	130.912020	21.019604	.33105057+02
38	145.357735	157.522171	.33027006+02	34	130.912024	-158.980394	.33105056+02

Total Coulomb Energy: 660.72530410

## 41 POINTS

D<sub>3vh</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
18	89.999999	.000001	.33850465+02	14	69.799365	-59.999999	.33922792+02
19	89.999999	120.000000	.33850464+02	15	69.799365	-179.999998	.33922791+02
24	90.000000	-119.999999	.33850464+02	16	69.799366	60.000001	.33922792+02
5	37.914060	-59.999999	.33903884+02	26	110.200634	-179.999998	.33922791+02
6	37.914060	-179.999998	.33903884+02	27	110.200635	60.000001	.33922792+02
7	37.914061	60.000001	.33903884+02	28	110.200635	-59.999999	.33922792+02
35	142.085937	179.999998	.33903884+02	17	89.999999	34.080736	.34017458+02
36	142.085939	60.000001	.33903884+02	20	89.999999	-34.080734	.34017458+02
37	142.085939	-59.999998	.33903884+02	21	89.999999	154.080736	.34017458+02
8	60.514777	20.670280	.33910697+02	22	89.999999	-85.919263	.34017458+02
9	60.514777	-20.670278	.33910697+02	23	90.000000	-154.080734	.34017458+02
10	60.514777	140.670280	.33910697+02	25	90.000001	85.919264	.34017458+02
11	60.514777	-99.329719	.33910697+02	1	.000000	.000000	.34024844+02
12	60.514778	99.329720	.33910697+02	41	179.999998	49.411086	.34024844+02
13	60.514778	-140.670277	.33910697+02	2	31.527829	120.000001	.34039874+02
29	119.485222	20.670280	.33910697+02	3	31.527830	.000000	.34039874+02
30	119.485222	-20.670278	.33910697+02	4	31.527830	-119.999998	.34039874+02
31	119.485222	-99.329719	.33910697+02	38	148.472170	.000001	.34039874+02
32	119.485222	-140.670279	.33910697+02	39	148.472170	119.999999	.34039874+02
33	119.485223	99.329721	.33910697+02	40	148.472170	-119.999999	.34039874+02
34	119.485223	140.670279	.33910697+02				

Total Coulomb Energy: 695.91674434

## 42 POINTS

D<sub>5vh</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
2	32.005909	-144.000002	.34801171+02	17	89.999999	-51.622373	.34863142+0
3	32.005909	-72.000001	.34801171+02	18	90.000000	20.377627	.34863142+0
4	32.005910	.000000	.34801171+02	19	90.000000	92.377627	.34863142+0
5	32.005910	71.999998	.34801171+02	20	90.000000	123.622370	.34863142+0
6	32.005910	143.999998	.34801171+02	21	90.000000	164.377626	.34863142+0
37	147.994089	143.999998	.34801171+02	22	90.000000	-164.377628	.34863142+0
38	147.994089	-72.000001	.34801171+02	23	90.000000	-123.622373	.34863142+0
39	147.994091	-.000003	.34801171+02	24	90.000000	-92.377630	.34863142+0
40	147.994091	71.999998	.34801171+02	25	90.000000	-20.377630	.34863142+0
41	147.994091	-144.000000	.34801171+02	26	90.000001	51.622370	.34863142+0
7	56.801032	-108.000001	.34820415+02	12	65.057714	-.000001	.34940347+0
8	56.801033	35.999999	.34820415+02	13	65.057714	-144.000002	.34940347+0
9	56.801033	107.999999	.34820415+02	14	65.057714	-72.000001	.34940347+0
10	56.801033	179.999998	.34820415+02	15	65.057715	71.999999	.34940347+0
11	56.801033	-36.000001	.34820415+02	16	65.057715	143.999998	.34940347+0
32	123.198967	179.999998	.34820415+02	27	114.942285	-.000001	.34940347+0
33	123.198967	-108.000001	.34820415+02	28	114.942285	143.999998	.34940347+0
34	123.198967	-36.000002	.34820415+02	29	114.942285	-144.000002	.34940347+0
35	123.198968	35.999998	.34820415+02	30	114.942285	-72.000002	.34940347+0
36	123.198968	107.999999	.34820415+02	31	114.942286	71.999999	.34940347+0
Total Coulomb Energy: 732.07810754				1	.000000	-90.000000	.34952730+0
				42	180.000000	-126.869898	.34952730+0

## 43 POINTS

 $C_{2v}$ 

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
42	162.854271	89.999996	.35702792+02	26	104.039161	119.410428	.35763813+02
43	162.854277	-90.000000	.35702792+02	27	104.039161	60.589568	.35763812+02
4	35.198014	-120.969164	.35725044+02	28	104.039162	-119.410432	.35763812+02
5	35.198014	-59.030839	.35725044+02	29	104.039162	-60.589570	.35763813+02
6	35.198015	59.030837	.35725044+02	34	124.581963	-90.000001	.35779419+02
7	35.198015	120.969160	.35725044+02	35	124.581966	89.999999	.35779419+02
10	59.408348	-21.462696	.35726126+02	30	118.067014	162.182390	.35793490+02
11	59.408349	-158.537308	.35726126+02	31	118.067014	17.817606	.35793490+02
12	59.408350	158.537304	.35726126+02	32	118.067015	-17.817617	.35793490+02
13	59.408350	21.462692	.35726126+02	33	118.067016	-162.182386	.35793490+02
20	90.197229	-90.000001	.35727639+02	36	135.534264	129.222187	.35808204+02
21	90.197230	89.999998	.35727639+02	37	135.534264	50.777808	.35808204+02
1	.000000	.000000	.35729368+02	38	135.534267	-129.222187	.35808203+02
18	86.645536	-.000002	.35736863+02	39	135.534267	-50.777816	.35808204+02
19	86.645537	179.999998	.35736863+02	22	90.388775	-32.082621	.35865845+02
14	69.931646	-57.510135	.35747032+02	23	90.388776	-147.917383	.35865845+02
15	69.931646	57.510130	.35747032+02	24	90.388778	147.917379	.35865845+02
16	69.931647	-122.489869	.35747032+02	25	90.388778	32.082617	.35865845+02
17	69.931647	122.489867	.35747032+02	8	58.817141	-90.000002	.35882231+02
40	150.676348	179.999996	.35748148+02	9	58.817142	89.999998	.35882231+02
41	150.676348	.000001	.35748148+02	2	31.721666	.000000	.35889965+02
				3	31.721667	179.999996	.35889965+02

Total Coulomb Energy: 769.19084646

## 44 POINTS

Octahedral

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
9	54.735599	44.999989	.36615764+02	3	22.395327	-44.999993	.36718711+02
10	54.735599	-135.000011	.36615764+02	4	22.395328	135.000006	.36718711+02
11	54.735621	-45.000011	.36615764+02	13	74.371183	73.754885	.36718711+02
12	54.735622	134.999989	.36615764+02	14	74.371183	-106.245115	.36718711+02
33	125.264378	-134.999979	.36615764+02	15	74.371192	-16.245104	.36718711+02
34	125.264379	45.000021	.36615764+02	16	74.371192	163.754894	.36718711+02
35	125.264401	135.000021	.36615764+02	17	74.371202	16.245106	.36718711+02
36	125.264401	-44.999979	.36615764+02	18	74.371202	-163.754894	.36718711+02
5	45.000000	90.000003	.36681112+02	19	74.371210	-73.754905	.36718711+02
6	45.000000	.000000	.36681112+02	20	74.371211	106.245095	.36718711+02
7	45.000000	180.000000	.36681112+02	25	105.628789	73.754915	.36718711+02
8	45.000000	-89.999996	.36681112+02	26	105.628790	-106.245084	.36718711+02
21	89.999997	-134.999994	.36681112+02	27	105.628798	-16.245095	.36718711+02
22	89.999998	45.000005	.36681112+02	28	105.628798	163.754906	.36718711+02
23	90.000002	-44.999995	.36681112+02	29	105.628808	16.245114	.36718711+02
24	90.000003	135.000006	.36681112+02	30	105.628809	-163.754885	.36718711+02
37	135.000000	.000010	.36681112+02	31	105.628816	-73.754874	.36718711+02
38	135.000000	90.000007	.36681112+02	32	105.628817	106.245126	.36718711+02
39	135.000000	-179.999989	.36681112+02	41	157.604671	-134.999996	.36718711+02
40	135.000000	-89.999993	.36681112+02	42	157.604673	45.000003	.36718711+02
1	22.395300	-134.999994	.36718711+02	43	157.604698	-44.999997	.36718711+02
2	22.395301	45.000007	.36718711+02	44	157.604700	135.000004	.36718711+02

Total Coulomb Energy: 807.17426308

## 45 POINTS

 $D_3$ 

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
1	19.159424	-119.999998	.37549214+02	40	141.843101	-5.765653	.37614161+02
2	19.159427	120.000009	.37549214+02	41	141.843163	-125.765647	.37614161+02
3	19.159428	.000000	.37549214+02	42	141.843166	114.234351	.37614161+02
43	160.840572	50.029913	.37549214+02	16	75.235791	-159.880997	.37638881+02
44	160.840572	170.029922	.37549214+02	17	75.235794	80.119004	.37638882+02
45	160.840574	-69.970082	.37549214+02	18	75.235802	-39.880992	.37638882+02
22	89.999997	25.014962	.37551586+02	28	104.764200	-150.089087	.37638882+02
23	89.999999	-94.985039	.37551586+02	29	104.764201	89.910915	.37638882+02
24	90.000003	145.014957	.37551586+02	30	104.764211	-30.089080	.37638881+02
19	79.502078	-126.285069	.37579025+02	7	48.969395	-141.765116	.37653604+02
20	79.502079	-6.285067	.37579025+02	8	48.969397	98.234882	.37653604+02
21	79.502081	113.714932	.37579025+02	9	48.969400	-21.765126	.37653604+02
25	100.497919	56.314988	.37579025+02	37	131.030602	-168.204954	.37653604+02
26	100.497920	-63.685010	.37579025+02	38	131.030602	71.795044	.37653604+02
27	100.497921	176.314987	.37579025+02	39	131.030605	-48.204966	.37653604+02
10	55.176860	16.874051	.37580118+02	13	68.949076	49.011216	.37672003+02
11	55.176863	136.874054	.37580119+02	14	68.949078	-70.988778	.37672003+02
12	55.176865	-103.125942	.37580118+02	15	68.949082	169.011211	.37672003+02
34	124.823134	-86.844136	.37580118+02	31	111.050919	-118.981298	.37672003+02
35	124.823139	153.155869	.37580118+02	32	111.050919	1.018710	.37672003+02
36	124.823140	33.155869	.37580118+02	33	111.050924	121.018702	.37672003+02
4	38.156835	-64.204431	.37614161+02	Total Coulomb Energy: 846.18840106			
5	38.156835	55.795573	.37614161+02				
6	38.156839	175.795570	.37614161+02				

46 POINTS  
Tetrahedral

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
11	57.902389	-135.262318	.38463763+02	8	54.735610	-60.000000	.38551855+02
12	57.902389	-15.262317	.38463763+02	9	54.735610	60.000000	.38551855+02
13	57.902389	104.737683	.38463763+02	10	54.735610	180.000000	.38551855+02
14	67.031726	-100.362006	.38463763+02	35	125.264390	-120.000000	.38551855+02
15	67.031726	139.637995	.38463763+02	36	125.264390	.000000	.38551855+02
16	67.031726	19.637994	.38463763+02	37	125.264390	120.000000	.38551855+02
23	88.506577	-124.960030	.38463763+02	1	.000000	.000000	.38572789+02
24	88.506577	115.039970	.38463763+02	32	109.471221	-180.000000	.38572789+02
25	88.506577	-4.960030	.38463763+02	33	109.471221	-60.000000	.38572789+02
44	161.378168	15.704317	.38463763+02	34	109.471221	60.000000	.38572789+02
45	161.378168	-104.295683	.38463763+02	2	29.805249	-154.685619	.38611643+02
46	161.378168	135.704317	.38463763+02	3	29.805249	85.314381	.38611643+02
5	36.051009	-97.063312	.38485588+02	4	29.805249	-34.685619	.38611643+02
6	36.051009	142.936687	.38485588+02	20	82.276839	-72.384906	.38611643+02
7	36.051009	22.936688	.38485588+02	21	82.276839	167.615093	.38611643+02
17	80.022912	-158.891405	.38485588+02	22	82.276839	47.615094	.38611643+02
18	80.022912	-38.891405	.38485588+02	29	109.118397	-148.378111	.38611643+02
19	80.022912	81.108595	.38485588+02	30	109.118397	91.621890	.38611643+02
26	101.611254	-96.601127	.38485588+02	31	109.118397	-28.378110	.38611643+02
27	101.611254	143.398872	.38485588+02	38	132.421963	157.469410	.38611643+02
28	101.611254	23.398873	.38485588+02	39	132.421963	-82.530590	.38611643+02
41	141.304306	-158.478537	.38485588+02	40	132.421963	37.469410	.38611643+02
42	141.304306	81.521463	.38485588+02	Total Coulomb Energy: 886.16711364			
43	141.304306	-38.478537	.38485588+02				

## 47 POINTS

C<sub>s</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
8	46.200496	-136.282768	.39338567+02	38	129.735386	53.288815	.39440564+02
9	46.200497	-43.717232	.39338567+02	39	129.735386	126.711192	.39440564+02
20	76.749602	-153.549564	.39356519+02	10	47.957292	90.000001	.39442235+02
21	76.749604	-26.450430	.39356519+02	29	104.348398	151.360880	.39444173+02
35	116.929681	90.000002	.39376945+02	30	104.348403	28.639122	.39444173+02
31	104.581723	-136.705645	.39384277+02	33	109.725728	-167.226786	.39462106+02
32	104.581730	-43.294347	.39384277+02	34	109.725733	-12.773205	.39462106+02
11	55.452680	.000000	.39387097+02	24	86.486025	90.000000	.39462218+02
12	55.452680	-180.000000	.39387097+02	40	131.185808	167.300770	.39495890+02
45	159.586227	-90.000009	.39391373+02	41	131.185818	12.699238	.39495890+02
25	99.371198	59.782067	.39403199+02	36	129.533342	-109.903776	.39504381+02
26	99.371198	120.217935	.39403199+02	37	129.533346	-70.096225	.39504381+02
46	161.977314	162.384258	.39412409+02	44	148.832865	90.000004	.39514401+02
47	161.977322	17.615747	.39412409+02	1	17.035803	-89.999999	.39516284+02
42	138.267414	-149.009689	.39418325+02	13	69.230386	64.513003	.39522684+02
43	138.267418	-30.990310	.39418325+02	14	69.230386	115.486999	.39522685+02
15	73.261449	147.284454	.39424711+02	22	85.745276	3.939737	.39523688+02
16	73.261452	32.715547	.39424710+02	23	85.745276	176.060266	.39523688+02
5	43.048596	137.128683	.39431333+02	3	25.645949	-176.597410	.39551050+02
6	43.048597	42.871314	.39431333+02	4	25.645951	-3.402592	.39551050+02
7	45.456363	-90.000001	.39432240+02	27	100.542883	-105.668252	.39551138+02
18	73.433030	-122.264637	.39433807+02	28	100.542887	-74.331739	.39551138+02
19	73.433034	-57.735355	.39433807+02	17	73.376712	-89.999994	.39580384+02
2	17.509057	89.999996	.39436623+02				

Total Coulomb Energy: 927.06226967



48 POINTS  
Octahedral

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
5	43.642961	115.069563	.40323478+02	1	21.243021	-18.630227	.40402643+02
6	43.642962	-64.930437	.40323478+02	2	21.243021	71.369772	.40402643+02
7	43.642962	-154.930437	.40323478+02	3	21.243021	161.369772	.40402643+02
8	43.642962	25.069563	.40323478+02	4	21.243022	-108.630228	.40402643+02
9	51.307174	-22.004016	.40323478+02	13	69.919582	-172.920902	.40402643+02
10	51.307174	-112.004015	.40323478+02	14	69.919582	-82.920902	.40402643+02
11	51.307175	157.995985	.40323478+02	15	69.919582	7.079098	.40402643+02
12	51.307175	67.995984	.40323478+02	16	69.919583	97.079098	.40402643+02
17	72.996243	-139.177183	.40323478+02	21	83.353233	-20.222214	.40402643+02
18	72.996243	-49.177183	.40323478+02	22	83.353234	69.777786	.40402643+02
19	72.996243	130.822817	.40323478+02	23	83.353234	-110.222214	.40402643+02
20	72.996243	40.822817	.40323478+02	24	83.353234	159.777786	.40402643+02
29	107.003757	-40.822817	.40323478+02	25	96.646766	-69.777785	.40402643+02
30	107.003757	139.177183	.40323478+02	26	96.646767	-159.777786	.40402643+02
31	107.003758	-130.822817	.40323478+02	27	96.646767	110.222214	.40402643+02
32	107.003758	49.177183	.40323478+02	28	96.646767	20.222214	.40402643+02
37	128.692825	-67.995985	.40323478+02	33	110.080417	172.920902	.40402643+02
38	128.692825	22.004015	.40323478+02	34	110.080417	-7.079098	.40402643+02
39	128.692825	112.004015	.40323478+02	35	110.080418	82.920903	.40402643+02
40	128.692825	-157.995985	.40323478+02	36	110.080418	-97.079098	.40402643+02
41	136.357038	-115.069563	.40323478+02	45	158.756977	-71.369773	.40402643+02
42	136.357038	64.930438	.40323478+02	46	158.756979	-161.369770	.40402643+02
43	136.357038	154.930437	.40323478+02	47	158.756979	108.630227	.40402643+02
44	136.357038	-25.069562	.40323478+02	48	158.756979	18.630228	.40402643+02

Total Coulomb Energy: 968.71345534

## 49 POINTS

C<sub>3</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
14	65.015594	-173.193148	.41216931+02	41	132.396736	10.666071	.41307614+02
15	65.015594	66.806854	.41216931+02	42	132.396738	-109.333928	.41307614+02
16	65.015594	-53.193147	.41216931+02	43	132.396738	130.666073	.41307614+02
23	84.609824	91.716971	.41219413+02	32	105.306824	-4.217718	.41321664+02
24	84.609824	-28.283029	.41219413+02	33	105.306825	115.782282	.41321664+02
25	84.609825	-148.283030	.41219413+02	34	105.306825	-124.217718	.41321664+02
17	77.671564	-114.627696	.41222953+02	35	115.393023	-153.662266	.41328549+02
18	77.671564	5.372304	.41222953+02	36	115.393023	86.337735	.41328549+02
19	77.671565	125.372304	.41222953+02	37	115.393023	-33.662265	.41328549+02
38	127.921910	170.938049	.41227191+02	8	52.515204	25.323908	.41334526+02
39	127.921910	-69.061951	.41227190+02	9	52.515204	-94.676091	.41334526+02
40	127.921911	50.938049	.41227190+02	10	52.515204	145.323910	.41334526+02
26	97.357410	61.594339	.41228158+02	44	144.324003	-30.841426	.41368313+02
27	97.357410	-58.405661	.41228158+02	45	144.324003	-150.841425	.41368313+02
28	97.357411	-178.405661	.41228158+02	46	144.324003	89.158574	.41368313+02
11	55.852836	-138.258211	.41231472+02	1	.000000	-45.000000	.41377957+02
12	55.852836	101.741790	.41231472+02	20	78.389992	-81.653624	.41380056+02
13	55.852836	-18.258211	.41231472+02	21	78.389993	158.346376	.41380056+02
5	35.333628	-177.251856	.41243831+02	22	78.389993	38.346376	.41380056+02
6	35.333628	-57.251856	.41243831+02	2	28.453771	-120.000001	.41400786+02
7	35.333628	62.748144	.41243831+02	3	28.453771	119.999999	.41400786+02
47	161.377239	151.980816	.41265566+02	4	28.453771	.000000	.41400786+02
48	161.377239	31.980814	.41265566+02	Total Coulomb Energy: 1011.55718265			
49	161.377239	-88.019183	.41265566+02				
29	105.075979	147.776848	.41281780+02				
30	105.075979	-92.223153	.41281780+02				
31	105.075979	27.776847	.41281780+02				

50 POINTS  
D<sub>6d</sub> (S<sub>12v</sub>)

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
1	.000000	90.000000	.42116966+02	2	31.637565	120.000000	.42225037+02
50	180.000000	-38.659808	.42116966+02	3	31.637566	-179.999998	.42225037+02
20	83.801461	150.000000	.42134813+02	4	31.637566	60.000000	.42225037+02
21	83.801461	90.000000	.42134813+02	5	31.637566	.000000	.42225037+02
22	83.801461	30.000000	.42134813+02	6	31.637566	-60.000000	.42225037+02
23	83.801461	-149.999998	.42134813+02	7	31.637566	-119.999998	.42225037+02
24	83.801462	-30.000000	.42134813+02	44	148.362434	90.000001	.42225037+02
25	83.801462	-90.000000	.42134814+02	45	148.362434	-150.000000	.42225037+02
26	96.198538	60.000000	.42134813+02	46	148.362434	150.000002	.42225037+02
27	96.198538	120.000000	.42134813+02	47	148.362434	30.000001	.42225037+02
28	96.198539	-180.000000	.42134813+02	48	148.362434	-30.000000	.42225037+02
29	96.198539	-119.999999	.42134814+02	49	148.362434	-90.000001	.42225037+02
30	96.198539	-60.000000	.42134813+02	8	54.130103	30.000001	.42289234+02
31	96.198540	.000000	.42134813+02	9	54.130103	150.000002	.42289234+02
14	67.487139	120.000001	.42195140+02	10	54.130103	-150.000000	.42289234+02
15	67.487139	60.000000	.42195140+02	11	54.130103	90.000000	.42289234+02
16	67.487139	-179.999998	.42195140+02	12	54.130104	-89.999999	.42289234+02
17	67.487140	-60.000000	.42195140+02	13	54.130104	-30.000000	.42289234+02
18	67.487140	.000000	.42195140+02	38	125.869896	-180.000000	.42289234+02
19	67.487140	-120.000000	.42195140+02	39	125.869896	120.000001	.42289234+02
32	112.512860	30.000001	.42195140+02	40	125.869897	-119.999999	.42289234+02
33	112.512860	150.000000	.42195140+02	41	125.869897	-59.999999	.42289234+02
34	112.512860	-149.999998	.42195140+02	42	125.869897	.000000	.42289234+02
35	112.512860	90.000000	.42195140+02	43	125.869897	60.000000	.42289234+02
36	112.512861	-29.999999	.42195140+02	Total Coulomb Energy: 1055.18231473			
37	112.512861	-90.000000	.42195140+02				

## 51 POINTS

D<sub>3</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
19	75.533971	55.664516	.43044064+02	34	108.739796	96.554500	.43151576+02
20	75.533972	175.664516	.43044064+02	35	108.739796	-143.445499	.43151576+02
21	75.533972	-64.335484	.43044064+02	36	108.739796	-23.445500	.43151576+02
31	104.466028	-55.664515	.43044064+02	7	46.886123	-79.818579	.43179738+02
32	104.466028	64.335485	.43044064+02	8	46.886124	40.181421	.43179738+02
33	104.466029	-175.664516	.43044064+02	9	46.886124	160.181421	.43179738+02
22	81.160383	-33.866610	.43050542+02	43	133.113876	-40.181420	.43179738+02
23	81.160383	-153.866610	.43050542+02	44	133.113876	-160.181419	.43179738+02
24	81.160383	86.133391	.43050542+02	45	133.113876	79.818580	.43179738+02
28	98.839616	33.866610	.43050542+02	4	35.032167	118.956536	.43187604+02
29	98.839617	153.866610	.43050542+02	5	35.032167	-121.043465	.43187604+02
30	98.839617	-86.133390	.43050542+02	6	35.032167	-1.043465	.43187604+02
10	50.872048	78.216453	.43095849+02	46	144.967833	121.043466	.43187604+02
11	50.872048	-161.783548	.43095849+02	47	144.967833	-118.956534	.43187604+02
12	50.872048	-41.783548	.43095849+02	48	144.967833	1.043465	.43187604+02
40	129.127951	41.783548	.43095849+02	25	90.000000	120.000000	.43190489+02
41	129.127953	-78.216451	.43095849+02	26	90.000000	-120.000000	.43190489+02
42	129.127953	161.783548	.43095849+02	27	90.000000	.000000	.43190489+02
1	18.189695	61.683524	.43102882+02	13	62.691515	-128.357746	.43198932+02
2	18.189695	-178.316477	.43102882+02	14	62.691515	111.642255	.43198932+02
3	18.189695	-58.316475	.43102882+02	15	62.691515	-8.357746	.43198932+02
49	161.810305	58.316476	.43102881+02	37	117.308485	-111.642254	.43198932+02
50	161.810305	178.316477	.43102881+02	38	117.308485	8.357746	.43198932+02
51	161.810305	-61.683523	.43102882+02	39	117.308485	128.357746	.43198932+02
16	71.260204	23.445501	.43151576+02	Total Coulomb Energy: 1099.81929032			
17	71.260204	143.445501	.43151576+02				
18	71.260204	-96.554499	.43151575+02				

## 52 POINTS

C<sub>3</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
17	75.318460	2.608658	.43957955+02	5	31.954733	-179.370661	.44062095+02
18	75.318460	-117.391342	.43957955+02	6	31.954733	-59.370660	.44062095+02
19	75.318462	122.608658	.43957955+02	7	31.954734	60.629340	.44062095+02
50	162.713406	-116.287587	.43980469+02	20	79.062328	36.437219	.44066491+02
51	162.713408	123.712412	.43980469+02	21	79.062328	-83.562782	.44066491+02
52	162.713408	3.712411	.43980469+02	22	79.062329	156.437220	.44066491+02
47	142.851511	-62.077983	.43986876+02	41	130.448805	18.355382	.44083555+02
48	142.851513	177.922018	.43986876+02	42	130.448805	-101.644618	.44083555+02
49	142.851513	57.922016	.43986876+02	43	130.448805	138.355383	.44083555+02
11	54.153936	99.328031	.43999750+02	38	113.191604	-161.026167	.44086390+02
12	54.153936	-140.671968	.43999750+02	39	113.191604	78.973835	.44086390+02
13	54.153936	-20.671970	.43999750+02	40	113.191604	-41.026166	.44086390+02
8	52.938250	144.635433	.44004847+02	1	.000000	135.000000	.44097264+02
9	52.938250	24.635434	.44004847+02	29	100.773854	18.370999	.44120787+02
10	52.938250	-95.364566	.44004847+02	30	100.773854	-101.629001	.44120787+02
23	82.331387	-147.911585	.44008132+02	31	100.773855	138.370998	.44120787+02
24	82.331387	-27.911583	.44008132+02	2	29.266884	-120.000002	.44145355+02
25	82.331388	92.088417	.44008132+02	3	29.266884	.000000	.44145355+02
14	59.876159	-56.199635	.44011048+02	4	29.266885	119.999999	.44145355+02
15	59.876160	63.800365	.44011048+02	44	135.355095	100.821409	.44155429+02
16	59.876160	-176.199635	.44011048+02	45	135.355095	-139.178591	.44155429+02
32	105.664463	-130.126425	.44027647+02	46	135.355095	-19.178591	.44155429+02
33	105.664463	-10.126424	.44027647+02	26	88.333472	-176.206032	.44161202+02
34	105.664464	109.873576	.44027648+02	27	88.333472	-56.206032	.44161201+02
35	112.785471	166.762514	.44055527+02	28	88.333473	63.793968	.44161201+02
36	112.785471	46.762514	.44055527+02				
37	112.785471	-73.237486	.44055527+02				
				Total Coulomb Energy: 1145.41896432			

## 53 POINTS

 $C_{2v}$ 

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
27	97.253574	-179.999994	.44860337+02	29	98.730293	116.985487	.44969386+02
28	97.253574	.000005	.44860337+02	30	98.730293	-63.014513	.44969386+02
7	43.995537	-.000002	.44868485+02	31	98.730296	63.014525	.44969387+02
8	43.995537	179.999998	.44868485+02	32	98.730296	-116.985475	.44969386+02
17	71.402469	164.609667	.44900419+02	13	65.531975	107.081566	.44992391+02
18	71.402469	-15.390335	.44900419+02	14	65.531975	-72.918434	.44992391+02
19	71.402474	-164.609665	.44900419+02	15	65.531983	72.918426	.44992391+02
20	71.402474	15.390335	.44900419+02	16	65.531984	-107.081574	.44992391+02
37	118.571793	90.000005	.44908846+02	53	180.000000	69.666441	.45030215+02
38	118.571794	-89.999995	.44908846+02	49	151.014032	-31.389861	.45039483+02
43	125.643970	-54.670184	.44915815+02	50	151.014032	148.610138	.45039483+02
44	125.643970	125.329816	.44915815+02	51	151.014038	31.389920	.45039484+02
45	125.643972	54.670197	.44915815+02	52	151.014038	-148.610081	.45039484+02
46	125.643972	-125.329803	.44915815+02	25	89.401688	-89.999994	.45043293+02
47	147.188236	90.000026	.44916662+02	26	89.401688	90.000006	.45043293+02
48	147.188238	-89.999974	.44916662+02	39	124.594347	-16.806341	.45044563+02
33	100.366344	149.127766	.44952878+02	40	124.594347	163.193659	.45044563+02
34	100.366344	-30.872234	.44952878+02	41	124.594369	-163.193668	.45044563+02
35	100.366368	-149.127764	.44952877+02	42	124.594369	16.806332	.45044563+02
36	100.366368	30.872237	.44952877+02	1	20.087706	136.915730	.45048956+02
9	47.918098	138.101519	.44955344+02	2	20.087706	-43.084271	.45048956+02
10	47.918098	-41.898482	.44955344+02	3	20.087728	43.084238	.45048956+02
11	47.918118	41.898477	.44955345+02	4	20.087728	-136.915762	.45048956+02
12	47.918118	-138.101522	.44955345+02	21	76.211505	135.010614	.45107742+02
5	39.884174	89.999991	.44955603+02	22	76.211506	-44.989385	.45107742+02
6	39.884174	-90.000009	.44955603+02	23	76.211527	-135.010620	.45107742+02
				24	76.211527	44.989379	.45107742+02

Total Coulomb Energy: 1191.92229042

## 54 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
51	153.437342	-13.755558	.45821743+02	49	140.354059	-66.956469	.45900356+02
52	153.437342	166.244442	.45821743+02	50	140.354059	113.043531	.45900356+02
23	81.144234	45.154913	.45831550+02	25	87.661751	100.566504	.45910284+02
24	81.144235	-134.845087	.45831550+02	26	87.661752	-79.433496	.45910284+02
7	43.808430	.000000	.45835227+02	31	98.239805	-28.854180	.45915216+02
8	43.808430	-180.000000	.45835227+02	32	98.239805	151.145821	.45915216+02
19	69.212096	17.027967	.45840302+02	39	116.038282	91.142733	.45919973+02
20	69.212096	-162.972033	.45840302+02	40	116.038283	-88.857267	.45919974+02
35	107.948433	-58.292827	.45845786+02	41	119.147546	-1.399454	.45921278+02
36	107.948433	121.707174	.45845786+02	42	119.147546	178.600546	.45921278+02
21	78.232573	130.941780	.45847729+02	37	112.771655	-128.853605	.45924997+02
22	78.232574	-49.058220	.45847729+02	38	112.771655	51.146394	.45924997+02
9	45.934203	137.290821	.45849603+02	5	38.234331	-94.693600	.45964615+02
10	45.934203	-42.709178	.45849603+02	6	38.234331	85.306400	.45964615+02
11	51.403299	-136.487474	.45851353+02	29	94.031302	-107.940803	.45968103+02
12	51.403299	43.512526	.45851353+02	30	94.031302	72.059197	.45968103+02
17	67.838373	-19.801197	.45856028+02	43	126.841755	-33.036190	.45988413+02
18	67.838374	160.198803	.45856028+02	44	126.841755	146.963810	.45988413+02
45	135.698084	-153.445034	.45863035+02	27	90.016528	-1.706819	.45992589+02
46	135.698084	26.554966	.45863035+02	28	90.016528	178.293180	.45992590+02
53	165.698343	-108.789910	.45864066+02	3	22.782320	36.414874	.45993472+02
54	165.698343	71.210092	.45864066+02	4	22.782320	-143.585127	.45993472+02
33	101.731802	-155.544376	.45870828+02	47	137.584339	-112.135101	.46001075+02
34	101.731802	24.455624	.45870828+02	48	137.584339	67.864900	.46001075+02
15	66.188863	-106.339928	.45881846+02	13	60.682102	106.882172	.46006803+02
16	66.188863	73.660073	.45881846+02	14	60.682103	-73.117829	.46006803+02
1	17.650802	-47.623885	.45895204+02	Total Coulomb Energy: 1239.36147473			
2	17.650802	132.376116	.45895204+02				

## 55 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
52	154.560356	178.374025	.46728238+02	8	50.392392	163.272560	.46821209+02
53	154.560356	-1.625975	.46728238+02	9	50.392393	-16.727439	.46821209+02
54	165.297707	-89.177995	.46751272+02	4	28.116587	-152.667812	.46832221+02
55	165.297707	90.822007	.46751272+02	5	28.116588	27.332188	.46832221+02
10	53.751097	-58.010466	.46753479+02	50	139.284882	-129.157782	.46834886+02
11	53.751097	121.989535	.46753479+02	51	139.284882	50.842218	.46834886+02
20	74.659844	145.576265	.46756588+02	38	111.898125	-72.043206	.46840372+02
21	74.659845	-34.423735	.46756588+02	39	111.898125	107.956794	.46840372+02
16	62.342894	-90.449607	.46756844+02	32	100.119672	12.885885	.46860860+02
17	62.342894	89.550393	.46756844+02	33	100.119672	-167.114115	.46860860+02
14	55.574311	-123.728369	.46760749+02	42	124.288154	163.895676	.46884853+02
15	55.574311	56.271632	.46760749+02	43	124.288154	-16.104326	.46884853+02
24	82.280359	117.364450	.46761940+02	28	89.883744	89.852108	.46892036+02
25	82.280359	-62.635550	.46761940+02	29	89.883744	-90.147892	.46892036+02
26	83.565202	-117.645084	.46762459+02	18	74.561071	-180.000000	.46904712+02
27	83.565202	62.354916	.46762459+02	19	74.561071	.000000	.46904712+02
34	105.672560	-43.830299	.46772245+02	1	.000000	97.125016	.46912227+02
35	105.672560	136.169701	.46772245+02	2	27.635434	-40.180007	.46925230+02
36	107.951143	43.223460	.46774632+02	3	27.635434	139.819990	.46925231+02
37	107.951143	-136.776539	.46774632+02	12	54.455636	-158.735010	.46928591+02
6	33.631046	-95.800697	.46774991+02	13	54.455636	21.264990	.46928591+02
7	33.631046	84.199303	.46774991+02	30	96.833591	163.385647	.46934061+02
48	137.337906	-47.759718	.46790106+02	31	96.833592	-16.614352	.46934061+02
49	137.337906	132.240280	.46790106+02	44	127.238136	-162.553043	.46944101+02
22	80.101551	-146.280586	.46797091+02	45	127.238136	17.446956	.46944101+02
23	80.101551	33.719414	.46797091+02	46	136.533985	-88.030087	.46963168+02
40	112.805388	-107.612353	.46809673+02	47	136.533985	91.969913	.46963168+02
41	112.805389	72.387647	.46809673+02				

Total Coulomb Energy 1287.77272078



## 56 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
33	101.300866	171.783377	.47681873+02	41	115.635216	-160.892572	.47748312+02
34	101.300880	-8.216634	.47681873+02	42	115.635224	19.107424	.47748313+02
49	139.319082	127.843325	.47682616+02	25	87.750701	-80.832355	.47748407+02
50	139.319098	-52.156682	.47682616+02	26	87.750703	99.167645	.47748408+02
9	45.194361	60.276650	.47687592+02	1	16.646390	60.741796	.47750696+02
10	45.194363	-119.723335	.47687592+02	2	16.646391	-119.258208	.47750696+02
47	132.245840	168.811689	.47689166+02	15	63.770336	122.947570	.47754535+02
48	132.245853	-11.188306	.47689167+02	16	63.770345	-57.052423	.47754535+02
23	79.966919	153.916496	.47691604+02	39	113.342551	111.676724	.47785159+02
24	79.966928	-26.083509	.47691604+02	40	113.342561	-68.323286	.47785159+02
35	101.496424	75.549611	.47698295+02	43	122.071729	52.797484	.47787263+02
36	101.496442	-104.450382	.47698294+02	44	122.071733	-127.202526	.47787263+02
7	41.488849	-163.103149	.47699373+02	53	155.327173	78.680435	.47787853+02
8	41.488850	16.896842	.47699373+02	54	155.327194	-101.319594	.47787853+02
17	65.982539	-144.753242	.47709011+02	5	37.954730	107.104326	.47798141+02
18	65.982545	35.246741	.47709011+02	6	37.954733	-72.895657	.47798141+02
11	50.664389	152.372353	.47716875+02	45	128.551632	86.002827	.47807978+02
12	50.664391	-27.627644	.47716875+02	46	128.551657	-93.997185	.47807978+02
55	164.291748	162.895884	.47720788+02	27	87.903637	-163.253185	.47825776+02
56	164.291761	-17.104057	.47720788+02	28	87.903649	16.746802	.47825777+02
31	95.500247	-135.736773	.47724210+02	13	62.420523	-90.180941	.47830131+02
32	95.500248	44.263218	.47724211+02	14	62.420528	89.819047	.47830131+02
19	66.556271	-179.999992	.47728503+02	3	23.111236	-24.830561	.47851607+02
20	66.556281	.000000	.47728503+02	4	23.111236	155.169439	.47851607+02
37	112.580595	144.760345	.47732338+02	29	90.089970	128.199821	.47858300+02
38	112.580612	-35.239664	.47732338+02	30	90.089984	-51.800181	.47858300+02
21	75.617843	64.263665	.47740583+02	51	143.166178	-151.802555	.47858362+02
22	75.617850	-115.736317	.47740582+02	52	143.166180	28.197466	.47858362+02

Total Coulomb Energy: 1337.09534827

## 57 POINTS

D<sub>3</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
1	16.382889	32.377728	.48629608+02	13	62.269242	100.475395	.48645710+02
2	16.382890	-87.622275	.48629608+02	14	62.269243	-19.524604	.48645710+02
3	16.382890	152.377729	.48629608+02	15	62.269243	-139.524605	.48645710+02
55	163.617109	147.622272	.48629608+02	43	117.730757	79.524605	.48645710+02
56	163.617109	27.622272	.48629608+02	44	117.730757	-160.475395	.48645710+02
57	163.617109	-92.377725	.48629608+02	45	117.730758	-40.475395	.48645710+02
16	65.368416	-50.501483	.48631090+02	28	90.000000	-30.000000	.48714745+02
17	65.368416	-170.501482	.48631090+02	29	90.000000	90.000000	.48714745+02
18	65.368416	69.498518	.48631090+02	30	90.000001	-150.000000	.48714745+02
40	114.631584	110.501482	.48631090+02	19	66.992795	-105.321040	.48723726+02
41	114.631584	-129.498516	.48631090+02	20	66.992795	14.678960	.48723726+02
42	114.631584	-9.498518	.48631090+02	21	66.992795	134.678961	.48723726+02
4	36.282140	-40.527125	.48635331+02	37	113.007205	165.321041	.48723726+02
5	36.282140	-160.527124	.48635331+02	38	113.007205	45.321040	.48723726+02
6	36.282140	79.472876	.48635332+02	39	113.007205	-74.678959	.48723726+02
52	143.717859	-19.472875	.48635332+02	7	40.221122	123.851299	.48746831+02
53	143.717861	100.527124	.48635331+02	8	40.221122	3.851300	.48746831+02
54	143.717861	-139.472876	.48635331+02	9	40.221123	-116.148700	.48746831+02
22	79.432445	39.848000	.48636262+02	49	139.778877	-63.851299	.48746831+02
23	79.432446	-80.152000	.48636262+02	50	139.778877	56.148701	.48746831+02
24	79.432446	159.848000	.48636262+02	51	139.778877	176.148701	.48746831+02
34	100.567554	20.152002	.48636262+02	25	87.201886	-3.339056	.48809568+02
35	100.567554	140.152000	.48636262+02	26	87.201887	-123.339057	.48809568+02
36	100.567555	-99.847999	.48636262+02	27	87.201887	116.660944	.48809568+02
10	49.261316	-77.720198	.48645577+02	31	92.798114	63.339056	.48809568+02
11	49.261316	42.279802	.48645577+02	32	92.798114	-176.660944	.48809568+02
12	49.261316	162.279800	.48645577+02	33	92.798114	-56.660944	.48809568+02
46	130.738684	17.720199	.48645577+02	Total Coulomb Energy: 1387.38322925			
47	130.738684	137.720200	.48645577+02				
48	130.738684	-102.279801	.48645577+02				

## 58 POINTS

D<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
12	53.886454	-86.324497	.49516198+02	48	129.640810	-132.274639	.49583425+02
13	53.886455	93.675502	.49516198+02	49	129.640812	47.725360	.49583425+02
46	126.113545	-21.964155	.49516198+02	4	29.473289	120.834150	.49599248+02
47	126.113545	158.035845	.49516198+02	5	29.473289	-59.165850	.49599249+02
24	80.168403	86.543210	.49531585+02	54	150.526711	-49.122802	.49599248+02
25	80.168403	-93.456790	.49531585+02	55	150.526712	130.877199	.49599249+02
34	99.831597	-14.831861	.49531585+02	20	75.824704	-147.967775	.49626026+02
35	99.831597	165.168139	.49531585+02	21	75.824704	32.032225	.49626026+02
18	71.669400	180.000000	.49549635+02	38	104.175296	39.679124	.49626025+02
19	71.669400	.000000	.49549636+02	39	104.175296	-140.320875	.49626026+02
40	108.330599	-108.288651	.49549636+02	8	49.579454	-18.229706	.49649348+02
41	108.330601	71.711349	.49549635+02	9	49.579455	161.770292	.49649348+02
26	80.193850	-64.132439	.49555456+02	50	130.420544	-90.058945	.49649348+02
27	80.193850	115.867560	.49555456+02	51	130.420546	89.941055	.49649348+02
32	99.806149	-44.156211	.49555456+02	14	56.428185	-52.248096	.49675144+02
33	99.806150	135.843788	.49555456+02	15	56.428186	127.751903	.49675144+02
16	57.566054	-120.538635	.49568939+02	44	123.571814	-56.040555	.49675144+02
17	57.566056	59.461365	.49568939+02	45	123.571816	123.959445	.49675144+02
42	122.433945	12.249982	.49568939+02	1	.000000	116.565051	.49685556+02
43	122.433945	-167.750017	.49568939+02	58	180.000000	136.169140	.49685556+02
22	76.307558	-30.266789	.49569421+02	28	84.208373	59.456728	.49694538+02
23	76.307559	149.733210	.49569421+02	29	84.208374	-120.543272	.49694538+02
36	103.692441	-78.021862	.49569421+02	30	95.791626	-167.745378	.49694538+02
37	103.692441	101.978138	.49569421+02	31	95.791626	12.254621	.49694538+02
6	30.777666	-115.810995	.49581390+02	2	26.501084	-175.881809	.49765994+02
7	30.777667	64.189006	.49581390+02	3	26.501084	4.118194	.49765994+02
52	149.222334	7.522343	.49581390+02	56	153.498917	-112.406844	.49765993+02
53	149.222334	-172.477655	.49581390+02	57	153.498917	67.593155	.49765994+02
10	50.359190	23.985988	.49583426+02				
11	50.359190	-156.014011	.49583425+02				
				Total Coulomb Energy: 1438.61825064			

## 59 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
1	.000000	-90.000000	.50433940+02	6	30.943528	-61.456603	.50528800+02
52	139.191219	-152.346161	.50441902+02	7	30.943528	118.543397	.50528800+02
53	139.191219	27.653840	.50441902+02	38	104.121280	-19.951050	.50533663+02
18	63.692918	-56.669307	.50448633+02	39	104.121280	160.048950	.50533663+02
19	63.692919	123.330693	.50448633+02	36	103.751866	-101.407369	.50536435+02
12	52.783912	-86.626906	.50464242+02	37	103.751866	78.592630	.50536435+02
13	52.783913	93.373094	.50464242+02	54	141.970057	-62.100967	.50557459+02
4	29.618686	-115.959982	.50471033+02	55	141.970057	117.899032	.50557459+02
5	29.618687	64.040017	.50471033+02	2	26.953536	177.908316	.50570592+02
40	112.336449	106.741445	.50482371+02	3	26.953537	-2.091684	.50570592+02
41	112.336449	-73.258556	.50482371+02	16	61.665538	180.000000	.50577172+02
24	77.098369	-25.878082	.50487733+02	17	61.665538	.000000	.50577172+02
25	77.098369	154.121920	.50487733+02	56	156.833521	67.423481	.50579312+02
46	118.930860	51.125110	.50492861+02	57	156.833523	-112.576519	.50579312+02
47	118.930861	-128.874889	.50492861+02	34	102.343487	28.848988	.50581306+02
30	89.078912	53.786407	.50494402+02	35	102.343487	-151.151012	.50581306+02
31	89.078912	-126.213593	.50494402+02	48	131.073303	80.437525	.50586055+02
58	164.573004	-18.319239	.50495851+02	49	131.073303	-99.562476	.50586055+02
59	164.573004	161.680761	.50495850+02	42	117.489368	6.038117	.50589746+02
32	91.583051	131.043381	.50499300+02	43	117.489368	-173.961884	.50589746+02
33	91.583051	-48.956620	.50499300+02	10	49.485114	-29.429284	.50603109+02
28	88.407747	3.216369	.50506339+02	11	49.485115	150.570717	.50603109+02
29	88.407748	-176.783630	.50506339+02	44	118.517019	-43.810436	.50621887+02
20	74.537865	29.409350	.50510028+02	45	118.517020	136.189564	.50621887+02
21	74.537866	-150.590651	.50510028+02	22	76.706558	79.259993	.50665305+02
50	137.157743	162.955345	.50516305+02	23	76.706559	-100.740007	.50665305+02
51	137.157745	-17.044655	.50516305+02	8	46.935894	-152.413013	.50676938+02
14	59.004391	57.716940	.50517883+02	9	46.935895	27.586987	.50676938+02
15	59.004391	-122.283060	.50517883+02	Total Coulomb Energy: 1490.77333528			
26	84.719970	-75.465001	.50519706+02				
27	84.719970	104.534998	.50519706+02				

## 60 POINTS

D<sub>3</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
1	16.048634	-175.519175	.51399556+02	13	62.144179	110.220095	.51435280+02
2	16.048634	64.480826	.51399556+02	14	62.144179	-129.779905	.51435281+02
3	16.048634	-55.519175	.51399556+02	15	62.144179	-9.779905	.51435280+02
58	163.951366	156.879675	.51399556+02	46	117.855820	-128.859594	.51435281+02
59	163.951366	-83.120326	.51399556+02	47	117.855821	111.140405	.51435281+02
60	163.951366	36.879674	.51399556+02	48	117.855821	-8.859595	.51435281+02
25	86.368103	123.606950	.51412732+02	19	66.843879	173.972912	.51473487+02
26	86.368104	-116.393050	.51412732+02	20	66.843879	53.972912	.51473487+02
27	86.368104	3.606950	.51412732+02	21	66.843879	-66.027088	.51473487+02
34	93.631896	-22.246451	.51412732+02	40	113.156121	167.387589	.51473487+02
35	93.631897	97.753549	.51412732+02	41	113.156121	47.387588	.51473487+02
36	93.631897	-142.246450	.51412732+02	42	113.156121	-72.612412	.51473487+02
28	86.986730	155.657202	.51421765+02	10	44.834728	80.388967	.51495536+02
29	86.986730	35.657201	.51421765+02	11	44.834729	-159.611032	.51495536+02
30	86.986730	-84.342799	.51421765+02	12	44.834729	-39.611032	.51495536+02
31	93.013270	-174.296701	.51421765+02	49	135.165272	140.971531	.51495536+02
32	93.013270	65.703299	.51421765+02	50	135.165272	-99.028467	.51495536+02
33	93.013270	-54.296701	.51421765+02	51	135.165272	20.971532	.51495536+02
16	63.506590	20.683264	.51424791+02	22	71.988757	-157.009081	.51552086+02
17	63.506591	140.683264	.51424791+02	23	71.988758	82.990920	.51552086+02
18	63.506591	-99.316737	.51424791+02	24	71.988758	-37.009080	.51552086+02
43	116.493409	-159.322763	.51424791+02	37	108.011242	138.369579	.51552086+02
44	116.493409	80.677237	.51424791+02	38	108.011242	18.369579	.51552086+02
45	116.493409	-39.322763	.51424791+02	39	108.011242	-101.630420	.51552086+02
4	34.672802	.000000	.51425921+02	7	41.752323	161.077084	.51568979+02
5	34.672803	-120.000000	.51425921+02	8	41.752323	41.077084	.51568979+02
6	34.672803	120.000000	.51425921+02	9	41.752323	-78.922916	.51568979+02
55	145.327196	-138.639502	.51425921+02	52	138.247677	60.283416	.51568979+02
56	145.327196	101.360499	.51425921+02	53	138.247677	-59.716584	.51568979+02
57	145.327198	-18.639500	.51425921+02	54	138.247679	-179.716583	.51568979+02

Total Coulomb Energy: 1543.83040098

61 POINTS  
C<sub>3</sub> (Non Min)

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
17	65.775180	-118.568699	.52304138+02	7	30.298248	61.282156	.52372993+02
19	65.854206	1.414094	.52304263+02	5	30.266336	-178.715111	.52373018+02
18	65.816932	121.394694	.52304332+02	6	30.271084	-58.657472	.52373287+02
16	57.405515	59.424091	.52308287+02	49	121.055577	20.660100	.52393529+02
15	57.386758	-60.508038	.52308599+02	47	120.985266	-99.373951	.52395778+02
14	57.375764	179.421169	.52308744+02	48	121.024160	140.649405	.52393860+02
44	115.784963	-128.967554	.52325181+02	32	92.908473	-108.434573	.52394497+02
46	115.870823	-8.963860	.52325390+02	33	92.946687	131.548452	.52394878+02
45	115.831660	111.040915	.52325515+02	34	92.983983	11.565085	.52395054+02
12	49.082836	-23.567702	.52337771+02	1	.000000	26.565051	.52407708+02
13	49.087329	96.371815	.52338089+02	22	73.058228	-35.103671	.52415968+02
11	49.074608	-143.622597	.52338217+02	21	73.057598	84.846906	.52416494+02
59	164.034100	-169.527300	.52342385+02	20	73.038586	-155.159037	.52416980+02
60	164.065027	-49.755664	.52342393+02	10	47.857760	24.961620	.52435278+02
61	164.108341	70.456158	.52342632+02	9	47.827452	144.954840	.52435637+02
57	145.783918	121.547468	.52345960+02	8	47.821577	-94.968082	.52436512+02
58	145.806923	1.488334	.52345994+02	43	115.438498	58.724491	.52463769+02
56	145.733088	-118.512976	.52346073+02	41	115.384954	178.732162	.52463792+02
27	85.400822	-59.361698	.52352743+02	42	115.403462	-61.288304	.52464203+02
28	85.422832	60.613530	.52353198+02	54	140.106657	166.238876	.52465049+02
26	85.391357	-179.403017	.52353480+02	53	140.105967	-73.842357	.52465403+02
25	73.099082	32.817787	.52354057+02	55	140.167309	46.232267	.52465458+02
24	73.072757	152.804281	.52354110+02	4	26.570044	-120.035317	.52478105+02
23	73.063261	-87.147111	.52354436+02	2	26.562757	119.913943	.52478436+02
38	103.103210	-156.510693	.52356470+02	3	26.564252	.000000	.52478928+02
39	103.148232	83.478575	.52356466+02	29	88.261291	-133.980453	.52488075+02
40	103.150518	-36.517666	.52356705+02	30	88.312839	105.999484	.52488622+02
50	132.797781	-154.607597	.52360716+02	31	88.352192	-13.979842	.52489088+02
52	132.852108	-34.649394	.52360823+02	35	99.420680	-82.516244	.52546181+02
51	132.849615	85.408733	.52360860+02	36	99.436381	157.407670	.52546244+02
				37	99.458039	37.485312	.52546469+02

Total Coulomb Energy: 1597.97266026

61 POINTS  
NO SYMMETRY

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
34	95.157148	46.494529	.52296308+02	35	97.292640	-33.007374	.52371006+02
36	100.232208	96.344580	.52309340+02	44	114.243843	-128.446932	.52372218+02
39	103.695604	-159.317982	.52313299+02	55	141.108440	-73.997944	.52376417+02
60	158.823891	109.125616	.52317416+02	21	70.473297	-31.634063	.52378866+02
9	41.443350	106.108636	.52317793+02	46	121.829830	-99.281116	.52384822+02
61	171.754616	-97.451488	.52320627+02	50	129.965530	99.160574	.52385231+02
42	112.183086	70.175185	.52328179+02	47	122.206794	38.874930	.52389608+02
32	93.168234	-109.435614	.52331320+02	20	68.517937	49.222239	.52391284+02
52	132.062473	7.253319	.52332219+02	31	88.780984	-57.954036	.52397831+02
6	37.699093	150.039452	.52332895+02	38	102.487890	19.208368	.52400156+02
53	136.897060	140.955456	.52334897+02	23	74.379906	-85.377540	.52401168+02
4	24.790361	4.608590	.52337284+02	7	39.035167	-123.534288	.52422995+02
18	63.493780	166.744919	.52337319+02	11	47.108660	-168.014145	.52429777+02
2	17.870837	-74.220842	.52338460+02	49	124.746435	-31.096734	.52445003+02
58	152.584249	-179.071733	.52339262+02	5	35.785717	59.004637	.52451114+02
22	71.649890	101.604832	.52340845+02	59	156.748299	29.253515	.52455121+02
26	81.692245	-5.636908	.52342897+02	37	100.840903	-82.836558	.52464510+02
30	88.304305	-136.678297	.52343814+02	29	87.628556	122.778173	.52468029+02
25	76.444141	-165.925676	.52344892+02	41	109.219177	149.895132	.52473659+02
48	123.073424	175.133858	.52345805+02	12	50.016162	25.939721	.52474332+02
15	60.685241	131.375650	.52346716+02	40	108.042298	-7.273612	.52481147+02
8	40.504492	-39.339633	.52347597+02	51	130.176933	-153.199970	.52486861+02
1	13.414991	97.804797	.52348322+02	27	82.770401	149.036888	.52490710+02
10	45.314727	-84.968856	.52348663+02	16	62.279765	-59.205173	.52501116+02
33	94.214936	174.331444	.52350552+02	14	58.325008	76.948483	.52503956+02
24	76.411172	21.153854	.52352557+02	57	150.289957	-30.033386	.52504137+02
28	85.200844	73.568122	.52353015+02	17	62.741280	-141.209785	.52506596+02
45	116.631866	-60.048853	.52353697+02	3	20.425870	-164.335602	.52512895+02
13	54.294366	-6.559202	.52353984+02	43	113.538089	122.168569	.52539069+02
56	145.367029	-120.198706	.52357165+02	54	139.087311	65.288869	.52540572+02
19	66.142531	-111.983364	.52366314+02				

Total Coulomb Energy: 1597.94183020

## 62 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
43	113.579608	-90.695126	.53224913+02	23	74.296293	4.909203	.53314772+02
44	113.579608	89.304874	.53224913+02	24	74.296293	-175.090797	.53314772+02
29	87.814793	-46.102767	.53240154+02	55	139.019522	103.032151	.53316930+02
30	87.814793	133.897232	.53240154+02	56	139.019522	-76.967849	.53316930+02
45	113.702304	-59.298922	.53256392+02	33	90.862787	26.880790	.53319150+02
46	113.702304	120.701078	.53256392+02	34	90.862787	-153.119209	.53319150+02
19	63.686348	-57.652403	.53260646+02	41	110.474934	151.416512	.53320431+02
20	63.686348	122.347597	.53260646+02	42	110.474934	-28.583489	.53320431+02
47	117.066546	29.626004	.53265510+02	49	128.879997	176.818916	.53326152+02
48	117.066546	-150.373997	.53265510+02	50	128.879997	-3.181083	.53326152+02
17	61.998016	31.691896	.53268761+02	13	60.185897	-114.587124	.53331431+02
18	61.998016	-148.308104	.53268761+02	14	60.185897	65.412876	.53331431+02
11	47.866323	-177.912771	.53281589+02	51	133.137686	65.207246	.53334459+02
12	47.866323	2.087228	.53281589+02	52	133.137686	-114.792754	.53334459+02
15	61.728069	153.318438	.53283645+02	59	159.324406	-19.061527	.53348534+02
16	61.728069	-26.681562	.53283645+02	60	159.324406	160.938473	.53348534+02
39	108.315554	56.962547	.53284101+02	1	15.169728	90.705065	.53354234+02
40	108.315554	-123.037453	.53284101+02	2	15.169728	-89.294935	.53354234+02
5	37.443773	-133.381433	.53284734+02	25	82.633355	-128.696016	.53398005+02
6	37.443773	46.618566	.53284734+02	26	82.633355	51.303983	.53398004+02
37	103.239090	2.336753	.53290425+02	57	143.459843	28.992310	.53419765+02
38	103.239090	-177.663246	.53290425+02	58	143.459843	-151.007690	.53419765+02
35	90.984341	-73.168167	.53295482+02	27	86.215956	160.953859	.53422017+02
36	90.984341	106.831833	.53295482+02	28	86.215956	-19.046140	.53422017+02
9	41.559822	-86.387061	.53295722+02	21	67.940250	-86.086929	.53422514+02
10	41.559822	93.612938	.53295721+02	22	67.940250	93.913071	.53422514+02
61	163.141806	-104.999998	.53295863+02	3	22.282858	.000000	.53433564+02
62	163.141806	75.000002	.53295863+02	4	22.282858	-180.000000	.53433564+02
31	89.385755	-102.288011	.53300953+02	53	135.576372	141.209995	.53435380+02
32	89.385755	77.711989	.53300953+02	54	135.576372	-38.790004	.53435380+02
7	38.461442	-43.804984	.53302369+02				
8	38.461442	136.195017	.53302369+02				

Total Coulomb Energy: 1652.92859368



63 POINTS  
D<sub>3</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
19	67.242562	23.338343	.54179804+02	37	97.638250	19.780280	.54238889+02
20	67.242562	143.338343	.54179804+02	38	97.638250	-100.219720	.54238889+02
21	67.242562	-96.661657	.54179804+02	39	97.638250	139.780279	.54238889+02
43	112.757438	115.248575	.54179804+02	31	90.000000	69.293459	.54244730+02
44	112.757438	-124.751425	.54179804+02	32	90.000000	-170.706541	.54244730+02
45	112.757438	-4.751425	.54179804+02	33	90.000000	-50.706541	.54244730+02
22	68.879792	88.871072	.54198598+02	16	64.400863	58.525328	.54246126+02
23	68.879792	-31.128928	.54198598+02	17	64.400863	-61.474672	.54246126+02
24	68.879792	-151.128927	.54198598+02	18	64.400863	178.525328	.54246126+02
40	111.120208	49.715847	.54198598+02	46	115.599137	80.061590	.54246126+02
41	111.120208	-70.284153	.54198598+02	47	115.599137	-39.938410	.54246126+02
42	111.120208	169.715845	.54198598+02	48	115.599137	-159.938410	.54246126+02
10	43.849478	157.781103	.54223153+02	13	56.318612	-4.612176	.54248679+02
11	43.849478	37.781104	.54223153+02	14	56.318612	115.387824	.54248679+02
12	43.849478	-82.218896	.54223153+02	15	56.318612	-124.612176	.54248679+02
52	136.150522	-19.194186	.54223153+02	49	123.681388	23.199094	.54248679+02
53	136.150522	100.805814	.54223153+02	50	123.681388	-96.800906	.54248679+02
54	136.150522	-139.194185	.54223153+02	51	123.681388	143.199095	.54248679+02
7	42.927849	79.127203	.54228348+02	28	85.631781	42.524847	.54333423+02
8	42.927849	-160.872797	.54228348+02	29	85.631781	-77.475153	.54333423+02
9	42.927849	-40.872797	.54228348+02	30	85.631781	162.524847	.54333423+02
55	137.072151	59.459715	.54228348+02	34	94.368219	96.062071	.54333423+02
56	137.072151	179.459715	.54228348+02	35	94.368219	-143.937929	.54333423+02
57	137.072151	-60.540285	.54228348+02	36	94.368219	-23.937929	.54333423+02
1	16.428515	-60.608213	.54238841+02	4	31.250230	.000000	.54368335+02
2	16.428515	59.391787	.54238841+02	5	31.250230	-120.000000	.54368335+02
3	16.428515	179.391787	.54238841+02	6	31.250230	120.000000	.54368335+02
61	163.571486	-40.804869	.54238841+02	58	148.749769	18.586918	.54368335+02
62	163.571486	79.195131	.54238841+02	59	148.749769	138.586918	.54368335+02
63	163.571486	-160.804869	.54238841+02	60	148.749769	-101.413082	.54368335+02
25	82.361750	118.806638	.54238889+02				
26	82.361750	-1.193362	.54238889+02				
27	82.361750	-121.193362	.54238889+02				

Total Coulomb Energy: 1708.87968150

64 POINTS  
C<sub>2</sub> (NONMINIMUM)

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
25	78.146083	147.782990	.55063911+02	41	108.781232	50.064058	.55163207+02
26	78.156790	-32.219309	.55063911+02	42	108.790799	-129.940037	.55163207+02
21	68.309229	20.863225	.55102437+02	13	52.473950	141.216045	.55166067+02
22	68.311709	-159.130762	.55102437+02	14	52.485879	-38.791480	.55166067+02
57	140.586529	97.253825	.55107045+02	7	37.468733	71.725975	.55178567+02
58	140.601938	-82.747633	.55107045+02	8	37.482169	-108.263959	.55178568+02
55	136.485462	58.246983	.55113340+02	61	154.607498	141.052254	.55179027+02
56	136.496662	-121.764200	.55113340+02	62	154.619436	-38.927103	.55179027+02
23	72.914727	118.768400	.55115269+02	17	61.090271	56.544586	.55181222+02
24	72.929512	-61.232967	.55115269+02	18	61.101218	-123.449304	.55181223+02
33	89.981596	97.835698	.55116864+02	35	95.143060	21.919894	.55207990+02
34	89.997047	-82.164282	.55116864+02	36	95.145815	-158.081493	.55207991+02
31	88.568287	70.723764	.55128984+02	15	60.052567	172.950430	.55208308+02
32	88.581527	-109.276034	.55128984+02	16	60.057468	-7.057942	.55208307+02
63	166.415428	65.347998	.55130106+02	3	23.802286	122.242601	.55211960+02
64	166.427860	-114.689959	.55130105+02	4	23.816722	-57.769872	.55211962+02
39	104.520674	152.570583	.55134553+02	49	122.667780	25.860068	.55222863+02
40	104.530407	-27.426290	.55134553+02	50	122.671548	-154.149496	.55222864+02
37	97.496313	126.894928	.55139670+02	47	114.610279	105.766744	.55272657+02
38	97.510299	-53.104181	.55139670+02	48	114.625718	-74.232715	.55272658+02
9	43.848177	30.448761	.55140781+02	27	83.021801	44.528218	.55275915+02
10	43.853220	-149.535952	.55140781+02	28	83.030167	-135.470234	.55275914+02
45	114.361012	77.913569	.55141636+02	59	147.727636	17.433484	.55279659+02
46	114.375142	-102.089229	.55141636+02	60	147.729158	-162.590853	.55279657+02
1	14.092225	36.671659	.55151117+02	11	48.691215	107.584415	.55285635+02
2	14.098840	-143.272715	.55151117+02	12	48.706582	-72.416930	.55285636+02
51	126.243960	132.433668	.55152157+02	53	131.527561	164.984509	.55289176+02
52	126.257246	-47.560493	.55152157+02	54	131.534487	-15.003220	.55289175+02
19	66.236497	85.720787	.55154010+02	5	34.733489	171.962950	.55291636+02
20	66.251373	-94.277269	.55154011+02	6	34.738628	-8.058134	.55291637+02
29	84.939807	174.958197	.55158253+02	43	110.087799	179.938427	.55356298+02
30	84.944196	-5.043081	.55158253+02	44	110.090889	-.056043	.55356298+02

Total Coulomb Energy:1765.82032131

64 POINTS  
D<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
31	88.412917	-103.226628	.55110216+02	19	65.669765	-82.610287	.55172783+02
32	88.412917	76.773372	.55110216+02	20	65.669765	97.389713	.55172783+02
33	91.587083	-76.773372	.55110216+02	45	114.330235	82.610287	.55172783+02
34	91.587083	103.226628	.55110216+02	46	114.330235	-97.389713	.55172783+02
9	45.055114	-61.634843	.55111560+02	15	57.567865	-28.560216	.55176333+02
10	45.055114	118.365157	.55111560+02	16	57.567865	151.439783	.55176333+02
55	134.944885	61.634843	.55111560+02	49	122.432135	-151.439783	.55176333+02
56	134.944885	-118.365157	.55111560+02	50	122.432135	28.560216	.55176333+02
21	72.445974	-55.200251	.55116738+02	1	13.106870	106.558362	.55182545+02
22	72.445974	124.799749	.55116738+02	2	13.106870	-73.441638	.55182545+02
43	107.554026	-124.799749	.55116738+02	63	166.893129	-106.558362	.55182545+02
44	107.554026	55.200251	.55116738+02	64	166.893129	73.441638	.55182545+02
7	37.615219	-100.277477	.55128726+02	27	80.326094	-130.030050	.55187286+02
8	37.615219	79.722523	.55128726+02	28	80.326094	49.969950	.55187286+02
57	142.384781	-79.722523	.55128726+02	37	99.673906	-49.969950	.55187286+02
58	142.384781	100.277477	.55128726+02	38	99.673906	130.030050	.55187286+02
25	77.612286	175.924686	.55130971+02	23	72.562213	-157.674761	.55225110+02
26	77.612286	-4.075314	.55130971+02	24	72.562213	22.325239	.55225110+02
39	102.387714	-175.924686	.55130971+02	41	107.437787	157.674761	.55225110+02
40	102.387714	4.075314	.55130971+02	42	107.437787	-22.325239	.55225110+02
13	51.547891	41.001842	.55147375+02	5	31.658929	-24.313098	.55294632+02
14	51.547891	-138.998158	.55147375+02	6	31.658929	155.686901	.55294632+02
51	128.452108	-41.001842	.55147375+02	59	148.341070	-155.686901	.55294632+02
52	128.452108	138.998158	.55147375+02	60	148.341070	24.313098	.55294632+02
11	50.872592	-175.299126	.55152467+02	17	62.338325	69.531013	.55295465+02
12	50.872592	4.700874	.55152467+02	18	62.338325	-110.468987	.55295465+02
53	129.127407	-4.700874	.55152467+02	47	117.661675	-69.531013	.55295465+02
54	129.127407	175.299126	.55152467+02	48	117.661675	110.468987	.55295465+02
3	26.274647	30.164729	.55163605+02	29	83.022241	-29.325195	.55305476+02
4	26.274647	-149.835272	.55163605+02	30	83.022241	150.674805	.55305476+02
61	153.725353	149.835272	.55163605+02	35	96.977759	-150.674805	.55305476+02
62	153.725353	-30.164729	.55163605+02	36	96.977759	29.325195	.55305476+02

Total Coulomb Energy: 1765.80257793

## 65 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
40	102.161726	-79.550124	.56022783+02	48	119.869609	-56.778434	.56106001+02
41	102.161726	100.449876	.56022783+02	49	119.869609	123.221566	.56106001+02
16	56.201350	-96.910455	.56033218+02	24	72.365401	180.000000	.56107105+02
17	56.201350	83.089545	.56033218+02	25	72.365401	.000000	.56107104+02
14	53.720811	-23.118381	.56034085+02	28	82.620287	-26.947175	.56116210+02
15	53.720811	156.881618	.56034085+02	29	82.620287	153.052826	.56116210+02
44	110.659166	-29.764965	.56041737+02	62	155.846817	-110.848538	.56129949+02
45	110.659166	150.235035	.56041737+02	63	155.846817	69.151462	.56129949+02
34	93.986192	-52.974656	.56043428+02	1	.000000	75.963757	.56135073+02
35	93.986192	127.025344	.56043428+02	10	47.361902	115.165268	.56137503+02
20	69.615709	-149.972689	.56045557+02	11	47.361902	-64.834732	.56137503+02
21	69.615709	30.027312	.56045557+02	30	84.182179	-99.396658	.56139739+02
6	28.788928	145.925882	.56051710+02	31	84.182179	80.603342	.56139739+02
7	28.788928	-34.074117	.56051710+02	46	116.623502	-147.587105	.56141753+02
56	136.836359	-23.412782	.56061286+02	47	116.623502	32.412895	.56141753+02
57	136.836359	156.587217	.56061286+02	12	48.507438	10.481379	.56148194+02
64	166.260820	-17.651731	.56062549+02	13	48.507438	-169.518621	.56148194+02
65	166.260820	162.348269	.56062549+02	54	130.699152	-122.803441	.56151368+02
42	107.089264	-110.147649	.56062709+02	55	130.699152	57.196559	.56151368+02
43	107.089264	69.852351	.56062709+02	22	72.146341	57.958536	.56169254+02
36	94.831787	46.969706	.56069516+02	23	72.146341	-122.041464	.56169254+02
37	94.831787	-133.030294	.56069516+02	50	120.596574	2.866399	.56169341+02
26	75.168860	105.426310	.56070237+02	51	120.596574	-177.133600	.56169341+02
27	75.168860	-74.573690	.56070237+02	60	145.346050	-62.025795	.56230410+02
4	28.212451	-94.664988	.56070580+02	61	145.346050	117.974205	.56230410+02
5	28.212451	85.335012	.56070580+02	18	67.932411	-48.136266	.56249655+02
8	47.087384	49.872425	.56087191+02	19	67.932411	131.863733	.56249655+02
9	47.087384	-130.127575	.56087191+02	2	25.190013	24.341204	.56274393+02
58	143.694786	-160.221889	.56097742+02	3	25.190013	-155.658796	.56274393+02
59	143.694786	19.778110	.56097742+02	38	97.558145	173.879486	.56275297+02
32	93.333124	-160.304873	.56099805+02	39	97.558145	-6.120514	.56275297+02
33	93.333124	19.695127	.56099805+02				
52	126.947617	-89.402417	.56100120+02				
53	126.947617	90.597583	.56100120+02				

Total Coulomb Energy: 1823.66796026

66 POINTS  
C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
59	142.942467	4.488175	.56966676+02	7	35.204451	143.847815	.57022003+02
60	142.942478	-175.511831	.56966675+02	8	35.204452	-36.152184	.57022003+02
31	87.785756	33.483379	.56968715+02	11	50.494362	101.447696	.57024359+02
32	87.785758	-146.516615	.56968715+02	12	50.494364	-78.552303	.57024358+02
57	137.599466	47.362733	.56969362+02	33	88.299961	166.451551	.57038498+02
58	137.599483	-132.637268	.56969362+02	34	88.299962	-13.548458	.57038498+02
3	25.119901	-86.514013	.56978581+02	13	51.868526	-111.763294	.57043545+02
4	25.119901	93.485982	.56978581+02	14	51.868529	68.236703	.57043545+02
21	70.930139	8.791262	.56989209+02	47	118.281898	-6.988382	.57049065+02
22	70.930141	-171.208733	.56989208+02	48	118.281900	173.011623	.57049065+02
55	132.523279	142.931686	.56989340+02	49	119.319246	23.639950	.57077064+02
56	132.523287	-37.068319	.56989340+02	50	119.319258	-156.360050	.57077065+02
45	108.985145	48.758998	.56995117+02	25	75.691280	-123.876969	.57078827+02
46	108.985156	-131.241007	.56995117+02	26	75.691284	56.123029	.57078827+02
53	125.671041	110.649972	.56998354+02	29	82.185021	140.159807	.57091067+02
54	125.671042	-69.350033	.56998354+02	30	82.185024	-39.840200	.57091067+02
9	43.551294	3.703650	.57004525+02	63	157.205879	137.294769	.57093802+02
10	43.551294	-176.296349	.57004525+02	64	157.205887	-42.705202	.57093802+02
51	121.391906	76.496895	.57006209+02	41	102.811115	122.627668	.57105095+02
52	121.391914	-103.503109	.57006208+02	42	102.811115	-57.372341	.57105095+02
65	165.677650	42.613432	.57007181+02	37	97.212856	10.277465	.57121467+02
66	165.677675	-137.386572	.57007181+02	38	97.212859	-169.722525	.57121467+02
17	59.631319	-146.076046	.57008263+02	5	33.772462	-138.068186	.57129221+02
18	59.631320	33.923953	.57008263+02	6	33.772464	41.931814	.57129221+02
27	78.222283	111.752411	.57008766+02	61	145.722185	88.554506	.57140465+02
28	78.222284	-68.247594	.57008766+02	62	145.722195	-91.445486	.57140464+02
23	73.983604	85.675134	.57010700+02	35	95.769855	70.734099	.57155670+02
24	73.983608	-94.324870	.57010700+02	36	95.769860	-109.265911	.57155670+02
1	12.920735	.000000	.57015309+02	43	107.586257	148.188206	.57158229+02
2	12.920735	-180.000000	.57015309+02	44	107.586263	-31.811804	.57158229+02
19	62.167789	160.910530	.57016123+02	15	58.325761	130.725035	.57164538+02
20	62.167790	-19.089472	.57016123+02	16	58.325763	-49.274967	.57164538+02
39	100.943922	96.237984	.57016184+02				
40	100.943924	-83.762026	.57016184+02				
				Total Coulomb Energy: 1882.44152547			

67 POINTS  
D<sub>5</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
22	71.454798	165.400551	.57922723+02	37	98.341226	25.933947	.57953609+02
23	71.454798	21.400551	.57922723+02	38	98.341226	-46.066053	.57953609+02
24	71.454798	-50.599449	.57922723+02	39	98.341226	97.933947	.57953609+02
25	71.454798	93.400551	.57922723+02	40	98.341226	-118.066053	.57953609+02
26	71.454798	-122.599449	.57922723+02	41	98.341226	169.933947	.57953609+02
42	108.545202	-93.400551	.57922723+02	7	42.678999	-135.832081	.57968991+02
43	108.545202	122.599449	.57922723+02	8	42.678999	8.167920	.57968991+02
44	108.545202	-165.400551	.57922723+02	9	42.678999	-63.832080	.57968991+02
45	108.545202	-21.400551	.57922723+02	10	42.678999	80.167920	.57968991+02
46	108.545202	50.599449	.57922723+02	11	42.678999	152.167919	.57968991+02
12	52.221152	-30.893580	.57934872+02	57	137.321001	135.832081	.57968991+02
13	52.221152	-102.893580	.57934872+02	58	137.321001	-8.167920	.57968991+02
14	52.221152	113.106420	.57934872+02	59	137.321001	63.832080	.57968991+02
15	52.221152	-174.893579	.57934872+02	60	137.321001	-80.167920	.57968991+02
16	52.221152	41.106420	.57934872+02	61	137.321001	-152.167919	.57968991+02
52	127.778848	30.893580	.57934872+02	32	90.000000	.000000	.57986089+02
53	127.778848	102.893580	.57934872+02	33	90.000000	72.000000	.57986089+02
54	127.778848	-113.106420	.57934872+02	34	90.000000	-72.000000	.57986089+02
55	127.778848	174.893579	.57934872+02	35	90.000000	144.000000	.57986089+02
56	127.778848	-41.106420	.57934872+02	36	90.000000	-144.000000	.57986089+02
2	25.495047	-27.041506	.57937950+02	1	.000000	-89.135447	.58054433+02
3	25.495047	44.958494	.57937950+02	7	180.000000	41.904867	.58054433+02
4	25.495047	-99.041506	.57937950+02	17	64.972118	-77.321966	.58102464+02
5	25.495047	116.958494	.57937950+02	18	64.972118	138.678034	.58102464+02
6	25.495047	-171.041506	.57937950+02	19	64.972118	-149.321966	.58102464+02
62	154.504953	27.041506	.57937950+02	20	64.972118	-5.321966	.58102464+02
63	154.504953	-44.958494	.57937950+02	21	64.972118	66.678034	.58102464+02
64	154.504953	99.041506	.57937950+02	47	115.027882	5.321966	.58102464+02
65	154.504953	-116.958494	.57937950+02	48	115.027882	77.321966	.58102464+02
66	154.504953	171.041506	.57937950+02	49	115.027882	-138.678034	.58102464+02
27	81.658774	-97.933947	.57953609+02	50	115.027882	149.321966	.58102464+02
28	81.658774	-169.933947	.57953609+02	51	115.027882	-66.678034	.58102464+02
29	81.658774	-25.933947	.57953609+02				
30	81.658774	46.066053	.57953609+02				
31	81.658774	118.066053	.57953609+02				

Total Coulomb Energy: 1942.12270041

## 68 POINTS

D<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
25	71.395104	-17.623424	.58819178+02	13	49.995581	79.071823	.58887218+02
26	71.395104	162.376575	.58819178+02	14	49.995581	-100.928177	.58887218+02
43	108.604896	17.623424	.58819178+02	55	130.004419	100.928177	.58887218+02
44	108.604896	-162.376575	.58819178+02	56	130.004419	-79.071823	.58887218+02
27	77.879893	85.955343	.58840120+02	29	84.093464	10.712740	.58887533+02
28	77.879893	-94.044657	.58840120+02	30	84.093464	-169.287260	.58887533+02
41	102.120107	-85.955343	.58840120+02	39	95.906536	-10.712740	.58887533+02
42	102.120107	94.044657	.58840120+02	40	95.906536	169.287260	.58887533+02
7	36.220565	116.757436	.58849907+02	19	62.738290	-45.159855	.58905874+02
8	36.220565	-63.242564	.58849907+02	20	62.738290	134.840145	.58905874+02
61	143.779434	63.242564	.58849907+02	49	117.261710	45.159855	.58905874+02
62	143.779434	-116.757436	.58849907+02	50	117.261710	-134.840145	.58905874+02
33	87.428080	-39.365333	.58860468+02	15	57.886781	5.864673	.58909295+02
34	87.428080	140.634666	.58860468+02	16	57.886781	-174.135326	.58909295+02
35	92.571920	39.365333	.58860468+02	53	122.113219	-5.864673	.58909295+02
36	92.571920	-140.634666	.58860468+02	54	122.113219	174.135326	.58909295+02
9	43.694622	-24.530677	.58870976+02	11	47.172258	45.071164	.59009419+02
10	43.694622	155.469322	.58870976+02	12	47.172258	-134.928837	.59009419+02
59	136.305378	24.530677	.58870976+02	57	132.827742	-45.071164	.59009419+02
60	136.305378	-155.469322	.58870976+02	58	132.827742	134.928837	.59009419+02
31	84.388410	114.326153	.58873051+02	5	32.996682	13.072040	.59020939+02
32	84.388410	-65.673847	.58873051+02	6	32.996682	-166.927959	.59020939+02
37	95.611590	65.673847	.58873051+02	63	147.003319	-13.072040	.59020939+02
38	95.611590	-114.326153	.58873051+02	64	147.003319	166.927959	.59020939+02
1	13.253641	-28.864066	.58881214+02	17	60.572626	106.461249	.59022395+02
2	13.253641	151.135935	.58881214+02	18	60.572626	-73.538751	.59022395+02
67	166.746359	28.864066	.58881214+02	51	119.427374	73.538751	.59022395+02
68	166.746359	-151.135935	.58881214+02	52	119.427374	-106.461249	.59022395+02
23	71.113729	59.642918	.58885851+02	21	69.081552	31.678866	.59028040+02
24	71.113729	-120.357082	.58885851+02	22	69.081552	-148.321135	.59028040+02
45	108.886271	-59.642918	.58885851+02	47	110.918448	-31.678866	.59028040+02
46	108.886271	120.357082	.58885851+02	48	110.918448	148.321135	.59028040+02
3	23.763282	68.421143	.58885873+02	Total Coulomb Energy: 2002.87470175			
4	23.763282	-111.578857	.58885873+02				
65	156.236717	111.578857	.58885873+02				
66	156.236717	-68.421143	.58885873+02				

## 69 POINTS

D<sub>3</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
10	43.530026	-154.801231	.59781010+02	61	140.215694	165.207224	.59837498+02
11	43.530026	85.198768	.59781010+02	62	140.215694	45.207224	.59837498+02
12	43.530026	-34.801231	.59781010+02	63	140.215694	-74.792777	.59837498+02
58	136.469975	124.375973	.59781010+02	22	68.761048	35.668022	.59847153+02
59	136.469975	-115.624027	.59781010+02	23	68.761048	155.668022	.59847153+02
60	136.469975	4.375974	.59781010+02	24	68.761049	-84.331977	.59847153+02
34	90.000000	104.787371	.59782069+02	46	111.238951	53.906719	.59847153+02
35	90.000000	-135.212629	.59782069+02	47	111.238952	173.906719	.59847153+02
36	90.000001	-15.212629	.59782068+02	48	111.238952	-66.093282	.59847153+02
28	79.060584	-110.852664	.59786790+02	25	75.402154	83.227204	.59870633+02
29	79.060584	129.147335	.59786790+02	26	75.402154	-156.772795	.59870633+02
30	79.060584	9.147336	.59786790+02	27	75.402155	-36.772796	.59870633+02
40	100.939416	80.427406	.59786790+02	43	104.597845	-113.652463	.59870633+02
41	100.939416	-159.572594	.59786790+02	44	104.597845	126.347537	.59870633+02
42	100.939417	-39.572594	.59786790+02	45	104.597846	6.347537	.59870633+02
1	15.545617	-177.228651	.59789206+02	4	30.159703	.000000	.59890208+02
2	15.545617	-57.228651	.59789206+02	5	30.159703	-120.000000	.59890207+02
3	15.545617	62.771349	.59789206+02	6	30.159703	120.000000	.59890208+02
67	164.454384	146.803391	.59789207+02	64	149.840298	89.574742	.59890208+02
68	164.454384	26.803394	.59789207+02	65	149.840298	-30.425258	.59890208+02
69	164.454384	-93.196608	.59789206+02	66	149.840298	-150.425259	.59890208+02
19	62.645035	-133.882799	.59800263+02	13	53.283907	-106.871648	.59916191+02
20	62.645035	106.117200	.59800263+02	14	53.283907	13.128351	.59916191+02
21	62.645036	-13.882801	.59800263+02	15	53.283907	133.128351	.59916191+02
49	117.354964	103.457542	.59800263+02	55	126.716093	76.446390	.59916191+02
50	117.354964	-136.542458	.59800263+02	56	126.716093	-163.553610	.59916191+02
51	117.354965	-16.542458	.59800263+02	57	126.716093	-43.553611	.59916191+02
31	86.393158	57.672821	.59807191+02	16	60.873751	62.006392	.59961511+02
32	86.393158	177.672821	.59807191+02	17	60.873751	-177.993608	.59961511+02
33	86.393159	-62.327179	.59807191+02	18	60.873751	-57.993608	.59961511+02
37	93.606841	31.901921	.59807191+02	52	119.126249	147.568350	.59961511+02
38	93.606842	151.901920	.59807191+02	53	119.126249	27.568350	.59961511+02
39	93.606842	-88.098079	.59807191+02	54	119.126250	-92.431651	.59961511+02
7	39.784306	164.367517	.59837498+02	Total Coulomb Energy: 2064.53606623			
8	39.784306	-75.632482	.59837498+02				
9	39.784306	44.367517	.59837498+02				



## 70 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
33	84.331039	-80.637405	.60670956+02	57	127.661598	79.497986	.60757578+02
34	84.331039	99.362595	.60670956+02	58	127.661598	-100.502014	.60757578+02
41	100.778162	4.388198	.60675466+02	65	144.025726	-33.752410	.60760531+02
42	100.778162	-175.611801	.60675466+02	66	144.025726	146.247589	.60760531+02
51	118.102221	-43.765380	.60681417+02	63	143.038307	50.597603	.60763655+02
52	118.102221	136.234619	.60681417+02	64	143.038307	-129.402397	.60763655+02
21	68.113003	-59.389606	.60716390+02	13	52.489109	61.744958	.60770875+02
22	68.113003	120.610394	.60716390+02	14	52.489109	-118.255042	.60770875+02
67	156.872555	-85.939075	.60718858+02	39	96.953423	31.007590	.60775468+02
68	156.872555	94.060925	.60718858+02	40	96.953423	-148.992411	.60775468+02
25	75.538441	74.084958	.60719290+02	29	79.624796	170.037889	.60779840+02
26	75.538441	-105.915042	.60719290+02	30	79.624796	-9.962110	.60779840+02
45	102.120773	-100.762683	.60729318+02	69	167.490013	4.613033	.60781115+02
46	102.120773	79.237317	.60729318+02	70	167.490013	-175.386967	.60781114+02
49	117.354945	-128.351917	.60730024+02	5	33.328567	-14.026315	.60794141+02
50	117.354945	51.648082	.60730024+02	6	33.328567	165.973684	.60794141+02
9	41.511946	-56.288000	.60735536+02	47	110.035160	104.259294	.60799389+02
10	41.511946	123.712000	.60735536+02	48	110.035160	-75.740706	.60799389+02
27	76.243998	16.957172	.60735586+02	17	57.323743	-30.426688	.60820911+02
28	76.243998	-163.042828	.60735586+02	18	57.323743	149.573313	.60820911+02
1	12.572046	-54.075296	.60745954+02	43	101.818143	-23.786272	.60822775+02
2	12.572046	125.924704	.60745954+02	44	101.818143	156.213728	.60822775+02
37	95.336014	-55.811730	.60746619+02	35	93.001282	56.028426	.60873969+02
38	95.336014	124.188270	.60746619+02	36	93.001282	-123.971574	.60873969+02
3	24.490838	35.906889	.60747896+02	7	33.473586	-95.279605	.60876379+02
4	24.490838	-144.093111	.60747896+02	8	33.473586	84.720395	.60876379+02
11	48.913126	29.165466	.60749115+02	59	133.788240	-68.550300	.60884322+02
12	48.913126	-150.834534	.60749115+02	60	133.788240	111.449700	.60884322+02
19	58.229765	94.625475	.60749651+02	15	56.247566	-180.000000	.60885292+02
20	58.229765	-85.374525	.60749651+02	16	56.247566	.000000	.60885292+02
23	71.781761	43.178589	.60753670+02	31	80.990821	-36.321653	.60915023+02
24	71.781761	-136.821411	.60753670+02	32	80.990821	143.678347	.60915022+02
53	120.620798	-157.442064	.60756349+02	61	142.991833	9.660123	.60946304+02
54	120.620798	22.557935	.60756349+02	62	142.991833	-170.339876	.60946304+02
55	122.984895	-11.010996	.60757013+02				
56	122.984895	168.989004	.60757013+02				

Total Coulomb Energy: 2127.12667460

## 71 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
28	77.899312	-105.352517	.61622177+02	22	68.336760	-51.342928	.61688938+02
29	77.899312	74.647483	.61622177+02	23	68.336760	128.657072	.61688938+02
26	72.290455	100.529113	.61626741+02	42	98.436472	164.439535	.61689006+02
27	72.290455	-79.470887	.61626741+02	43	98.436472	-15.560465	.61689006+02
1	.000000	135.000000	.61636377+02	48	111.199719	-140.191404	.61693983+02
38	93.104213	-63.136837	.61640864+02	49	111.199719	39.808596	.61693983+02
39	93.104213	116.863163	.61640864+02	60	131.610182	-123.471730	.61694109+02
6	27.457105	65.103586	.61646197+02	61	131.610182	56.528270	.61694109+02
7	27.457105	-114.896414	.61646197+02	56	124.303793	164.972101	.61703038+02
16	53.461179	-179.907194	.61647777+02	57	124.303793	-15.027899	.61703038+02
17	53.461179	.092805	.61647776+02	50	113.566323	-40.998616	.61709669+02
10	46.414420	147.880079	.61651507+02	51	113.566323	139.001385	.61709669+02
11	46.414420	-32.119921	.61651507+02	46	109.590345	-172.040400	.61713564+02
52	118.131536	-68.215267	.61663712+02	47	109.590345	7.959600	.61713564+02
53	118.131536	111.784733	.61663712+02	32	84.940842	-131.555386	.61716621+02
4	26.273731	-180.000000	.61663930+02	33	84.940842	48.444615	.61716622+02
5	26.273731	.000000	.61663930+02	20	67.408162	-154.384857	.61753643+02
14	51.006103	-99.587079	.61665361+02	21	67.408162	25.615143	.61753643+02
15	51.006103	80.412921	.61665361+02	18	60.728093	53.997357	.61781919+02
44	103.067148	-114.637303	.61666933+02	19	60.728093	-126.002643	.61781919+02
45	103.067148	65.362697	.61666933+02	12	48.549905	-68.331078	.61809045+02
30	80.367083	-178.383802	.61670372+02	13	48.549905	111.668922	.61809045+02
31	80.367083	1.616198	.61670372+02	66	148.276121	-7.723027	.61811982+02
58	131.597212	21.437130	.61673256+02	67	148.276121	172.276974	.61811982+02
59	131.597212	-158.562870	.61673256+02	2	25.228626	-59.157565	.61812570+02
62	138.731783	-47.423996	.61674009+02	3	25.228626	120.842435	.61812570+02
63	138.731783	132.576004	.61674009+02	54	120.662258	-96.003142	.61822484+02
70	167.350779	126.552008	.61676492+02	55	120.662258	83.996858	.61822484+02
71	167.350779	-53.447992	.61676492+02	8	42.922224	-147.555061	.61823542+02
68	156.014885	44.791099	.61678829+02	9	42.922224	32.444939	.61823542+02
69	156.014885	-135.208900	.61678829+02	34	89.541862	-38.562370	.61841870+02
64	144.432446	-86.373119	.61679823+02	35	89.541862	141.437630	.61841870+02
65	144.432446	93.626881	.61679823+02	36	91.881591	-155.778172	.61849918+02
40	96.748318	91.965923	.61680225+02	37	91.881591	24.221829	.61849918+02
41	96.748318	-88.034077	.61680225+02				
24	70.435016	157.737146	.61687613+02				
25	70.435016	-22.262853	.61687613+02				

Total Coulomb Energy: 2190.64990643

72 POINTS  
ICOSAHERAL

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
2	24.491708	39.825982	.62614943+02	42	102.094709	32.969481	.62614943+02
3	24.491708	-176.174019	.62614943+02	43	102.094709	176.969481	.62614943+02
4	24.491708	111.825982	.62614943+02	44	102.094709	-39.030519	.62614943+02
5	24.491708	-32.174018	.62614943+02	45	102.094709	-111.030519	.62614943+02
6	24.491708	-104.174018	.62614943+02	46	102.094709	104.969481	.62614943+02
7	41.306485	148.496859	.62614943+02	47	112.472011	-63.408424	.62614943+02
8	41.306485	4.496859	.62614943+02	48	112.472011	152.591576	.62614943+02
9	41.306485	-67.503141	.62614943+02	49	112.472011	8.591576	.62614943+02
10	41.306485	-139.503141	.62614943+02	50	112.472011	80.591576	.62614943+02
11	41.306485	76.496859	.62614943+02	51	112.472011	-135.408424	.62614943+02
12	49.875354	42.606076	.62614943+02	57	130.124645	29.393924	.62614943+02
13	49.875354	-173.393925	.62614943+02	58	130.124645	-42.606076	.62614943+02
14	49.875354	-29.393924	.62614943+02	59	130.124645	-114.606076	.62614943+02
15	49.875354	-101.393924	.62614943+02	60	130.124645	173.393925	.62614943+02
16	49.875354	114.606076	.62614943+02	61	130.124645	101.393924	.62614943+02
22	67.527989	63.408424	.62614943+02	62	138.693516	67.503141	.62614943+02
23	67.527989	-80.591576	.62614943+02	63	138.693516	-76.496859	.62614943+02
24	67.527989	-8.591576	.62614943+02	64	138.693516	139.503141	.62614943+02
25	67.527989	-152.591576	.62614943+02	65	138.693516	-4.496859	.62614943+02
26	67.527989	135.408424	.62614943+02	66	138.693516	-148.496859	.62614943+02
27	77.905291	39.030519	.62614943+02	67	155.508291	32.174018	.62614943+02
28	77.905291	-176.969481	.62614943+02	68	155.508291	104.174018	.62614943+02
29	77.905291	-104.969481	.62614943+02	69	155.508291	-39.825982	.62614943+02
30	77.905291	-32.969481	.62614943+02	70	155.508291	176.174019	.62614943+02
31	77.905291	111.030519	.62614943+02	71	155.508291	-111.825982	.62614943+02
32	87.279315	84.167114	.62614943+02	1	.000000	.000000	.62758816+02
33	87.279315	156.167114	.62614943+02	17	63.434949	18.000000	.62758816+02
34	87.279315	-59.832886	.62614943+02	18	63.434949	-54.000000	.62758816+02
35	87.279315	12.167114	.62614943+02	19	63.434949	162.000000	.62758816+02
36	87.279315	-131.832886	.62614943+02	20	63.434949	90.000000	.62758816+02
37	92.720685	-12.167114	.62614943+02	21	63.434949	-126.000000	.62758816+02
38	92.720685	59.832886	.62614943+02	52	116.565051	54.000000	.62758816+02
39	92.720685	131.832886	.62614943+02	53	116.565051	126.000000	.62758816+02
40	92.720685	-156.167114	.62614943+02	54	116.565051	-90.000000	.62758816+02
41	92.720685	-84.167114	.62614943+02	55	116.565051	-18.000000	.62758816+02
Total Coulomb Energy: 2255.00119097				56	116.565051	-162.000000	.62758816+02
				72	180.000000	-7.587135	.62758816+02

## 73 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
16	53.773001	-104.424023	.63450505+02	58	124.344561	90.507773	.63565898+02
17	53.773001	75.575977	.63450505+02	59	124.344561	-89.492227	.63565898+02
12	47.139684	-69.944919	.63481396+02	22	67.536679	-130.377274	.63565965+02
13	47.139684	110.055081	.63481396+02	23	67.536679	49.622727	.63565965+02
18	62.377893	-159.326817	.63484079+02	24	68.890939	125.892529	.63568247+02
19	62.377893	20.673183	.63484079+02	25	68.890939	-54.107471	.63568247+02
44	98.532284	163.004269	.63496416+02	40	96.832199	-43.373466	.63580690+02
45	98.532284	-16.995731	.63496416+02	41	96.832199	136.626534	.63580690+02
4	26.076245	138.106379	.63506252+02	50	111.766576	-141.401646	.63583542+02
5	26.076245	-41.893622	.63506252+02	51	111.766576	38.598355	.63583542+02
30	79.887473	-105.716663	.63517826+02	48	109.549668	-111.713684	.63592033+02
31	79.887473	74.283337	.63517826+02	49	109.549668	68.286316	.63592033+02
42	98.281121	-89.122331	.63523131+02	10	44.361792	-136.702024	.63594419+02
43	98.281121	90.877669	.63523131+02	11	44.361792	43.297975	.63594419+02
6	28.841530	-97.779448	.63526421+02	32	84.885505	-176.680428	.63607945+02
7	28.841530	82.220552	.63526421+02	33	84.885505	3.319572	.63607945+02
66	145.058779	162.888111	.63527382+02	46	106.818961	-166.813837	.63611433+02
67	145.058779	-17.111888	.63527382+02	47	106.818961	13.186163	.63611433+02
14	50.275687	145.268213	.63530796+02	28	76.981741	150.346483	.63620350+02
15	50.275687	-34.731787	.63530796+02	29	76.981741	-29.653516	.63620350+02
26	70.100972	-82.424186	.63531467+02	8	42.082699	.000000	.63632590+02
27	70.100972	97.575814	.63531467+02	9	42.082699	180.000000	.63632590+02
34	85.856143	-151.296967	.63544587+02	56	121.358631	172.248552	.63665945+02
35	85.856143	28.703033	.63544587+02	57	121.358631	-7.751447	.63665945+02
62	132.846689	-159.475508	.63545692+02	36	89.643826	-66.814355	.63670980+02
63	132.846689	20.524492	.63545692+02	37	89.643826	113.185645	.63670980+02
64	139.234762	122.937029	.63547542+02	1	.000000	90.000000	.63686367+02
65	139.234762	-57.062971	.63547542+02	18	148.383789	84.243761	.63700848+02
72	167.394199	129.336149	.63548367+02	69	148.383789	-95.756239	.63700848+02
73	167.394199	-50.663850	.63548367+02	20	64.725742	-8.490646	.63708832+02
52	114.241551	-64.283699	.63549661+02	21	64.725742	171.509354	.63708832+02
53	114.241551	115.716301	.63549661+02	38	91.470516	-127.309779	.63720848+02
70	156.678600	-147.907631	.63557379+02	39	91.470516	52.690221	.63720848+02
71	156.678600	32.092369	.63557379+02	2	22.810388	-155.314896	.63810099+02
54	120.294757	144.150743	.63558967+02	3	22.810388	24.685104	.63810099+02
55	120.294757	-35.849257	.63558966+02				
60	132.179621	-124.526083	.63562169+02				
61	132.179621	55.473917	.63562169+02				

Total Coulomb Energy: 2320.63388375

74 POINTS  
D<sub>2</sub> (NONMIN)

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
16	53.501831	72.891611	.64400558+02	48	110.259631	70.608391	.64498492+02
17	53.573448	-107.027818	.64400559+02	49	110.326740	-109.432979	.64498493+02
58	126.405683	92.153833	.64400766+02	26	69.645323	94.477588	.64498862+02
59	126.509171	-87.904851	.64400766+02	27	69.751995	-85.494632	.64498863+02
44	98.652104	91.758382	.64434710+02	34	86.359708	-175.446306	.64503251+02
45	98.755075	-88.253885	.64434710+02	35	86.434687	4.546965	.64503252+02
30	81.240907	73.317513	.64435513+02	40	93.549577	160.514071	.64503302+02
31	81.313271	-106.665829	.64435513+02	41	93.661540	-19.481712	.64503303+02
18	62.820736	-161.243437	.64435641+02	22	67.237107	169.797743	.64520844+02
19	62.867281	18.694038	.64435642+02	23	67.336823	-10.237468	.64520845+02
56	117.119132	146.332947	.64435889+02	52	112.678527	175.251736	.64521228+02
57	117.244077	-33.647788	.64435888+02	53	112.769738	-4.709195	.64521228+02
6	27.780540	74.987504	.64463451+02	66	135.747124	166.869274	.64549019+02
7	27.856208	-104.811103	.64463451+02	67	135.850929	-13.049479	.64549018+02
68	152.122252	90.022702	.64463504+02	8	44.178896	178.229429	.64549172+02
69	152.222639	-90.135124	.64463503+02	9	44.265252	-1.871050	.64549174+02
10	44.785155	39.944917	.64466052+02	1	.065237	-50.366680	.64562813+02
11	44.786012	-139.923649	.64466051+02	74	179.934763	129.628519	.64563000+02
64	135.147169	125.042370	.64466156+02	32	84.264217	-149.946487	.64573417+02
65	135.277206	-54.968156	.64466155+02	33	84.285925	30.040609	.64573417+02
50	112.270675	115.388082	.64471460+02	42	95.687880	135.027510	.64573663+02
51	112.397119	-64.625114	.64471460+02	43	95.817758	-44.971261	.64573663+02
24	67.648736	49.644345	.64471550+02	36	87.115955	112.627202	.64610342+02
25	67.671474	-130.302866	.64471550+02	37	87.240709	-67.370926	.64610342+02
62	135.034061	59.618445	.64478518+02	38	92.791535	52.467841	.64611359+02
63	135.078520	-120.504450	.64478518+02	39	92.820506	-127.538383	.64611359+02
12	44.869664	105.466330	.64479123+02	54	114.997873	43.345272	.64614953+02
13	44.988710	-74.480186	.64479124+02	55	115.006246	-136.715443	.64614953+02
70	154.630003	-149.358648	.64480824+02	20	64.904492	121.751261	.64615448+02
71	154.650076	30.913303	.64480823+02	21	65.033722	-58.240390	.64615448+02
4	25.300432	134.290388	.64480952+02	28	73.775908	145.284300	.64615683+02
5	25.430459	-45.731898	.64480954+02	29	73.901536	-34.725894	.64615684+02
14	48.411743	144.690428	.64482145+02	46	106.152701	-160.250145	.64616350+02
15	48.537731	-35.339561	.64482146+02	47	106.197020	19.785450	.64616351+02
60	131.503397	-159.638622	.64482577+02	72	156.254446	147.680731	.64666759+02
61	131.546326	20.470454	.64482577+02	73	156.378452	-32.226892	.64666758+02
Total Coulomb Energy: 2387.10121441				2	23.660707	-162.575119	.64666771+02
				3	23.710305	17.149836	.64666772+02

74 POINTS  
NONSYM (MIN)

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
45	100.958158	15.494045	.64381019+02	69	146.155437	52.801339	.64506184+02
23	66.646088	104.020895	.64410851+02	43	99.150776	-11.697996	.64507728+02
65	141.370668	-145.652849	.64412923+02	5	30.751582	46.826215	.64508707+02
52	114.846775	-32.699345	.64414071+02	4	28.961789	-76.430786	.64512729+02
55	120.465643	-89.285508	.64416965+02	72	163.367182	100.913124	.64513186+02
58	122.229063	60.953401	.64427259+02	9	39.481445	-38.229579	.64516214+02
1	10.636145	-18.538446	.64428529+02	56	120.481597	-1.821267	.64517199+02
15	54.107744	-69.573041	.64432406+02	28	77.301029	126.965903	.64519722+02
41	98.898593	-105.803061	.64433911+02	11	44.501329	81.541761	.64522592+02
46	101.112595	136.616682	.64438769+02	64	138.258532	-27.319444	.64527344+02
60	124.622187	149.908361	.64441579+02	12	44.669211	116.160378	.64529714+02
53	117.244138	-149.364956	.64445385+02	68	142.564835	-103.922336	.64530149+02
13	51.606089	-101.065084	.64453923+02	70	151.583731	168.092560	.64534370+02
17	55.564169	19.905161	.64459245+02	44	99.417933	-130.564392	.64534845+02
57	121.679258	-119.937727	.64460464+02	39	95.251033	111.107519	.64536939+02
26	75.341898	-112.740024	.64462272+02	37	91.215397	-39.991701	.64538625+02
20	58.478634	170.615244	.64462539+02	49	106.101063	-59.302919	.64543060+02
51	112.761798	90.106606	.64463526+02	42	98.991031	67.835335	.64548683+02
3	20.359321	101.109937	.64463611+02	14	53.690241	-133.327209	.64553740+02
35	82.294581	178.750259	.64464075+02	38	91.271170	-156.204700	.64557175+02
33	79.609764	-62.639084	.64464742+02	48	103.264461	161.828062	.64557259+02
10	40.757547	-165.181623	.64465023+02	40	97.156335	-81.719362	.64570893+02
34	80.261769	153.270794	.64466888+02	24	67.504621	75.788828	.64578426+02
16	55.235645	48.969291	.64466962+02	18	55.810588	-11.055628	.64578942+02
59	122.964460	30.437169	.64469479+02	2	14.021387	-170.218290	.64589638+02
30	78.130422	4.800891	.64470535+02	73	165.635860	-.581403	.64600155+02
22	65.502190	-161.500216	.64470959+02	36	87.244432	88.959696	.64603366+02
54	118.923008	117.732233	.64475866+02	19	57.913416	141.625166	.64603773+02
31	78.771063	29.621313	.64477850+02	32	79.313730	54.065981	.64605567+02
47	101.537999	41.801272	.64479341+02	7	33.528290	2.686224	.64635636+02
8	34.570706	153.983776	.64487335+02	66	141.717752	126.729189	.64643968+02
63	136.600702	89.658465	.64490016+02	71	152.825514	-63.425812	.64645545+02
61	129.160152	-61.410865	.64493374+02	6	30.808846	-123.867130	.64665178+02
62	129.542088	-179.085669	.64499514+02	50	106.749421	-174.140356	.64666952+02
21	63.808934	-42.459758	.64500862+02	67	142.472912	11.010293	.64689936+02
74	166.306772	-133.184517	.64501615+02	27	76.614311	-137.229357	.64708652+02
25	73.927917	-87.916512	.64503033+02	29	77.457316	-20.799214	.64715069+02

Total Coulomb Energy: 2387.08728748

## 75 POINTS

D<sub>3</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
31	79.324149	-50.111120	.65340894+02	55	120.090583	104.473278	.65441766+02
32	79.324150	69.888874	.65340895+02	56	120.090586	-15.526722	.65441766+02
33	79.324157	-170.111118	.65340892+02	57	120.090590	-135.526712	.65441766+02
43	100.675843	86.559062	.65340894+02	1	14.596205	-82.009245	.65451979+02
44	100.675846	-33.440932	.65340894+02	2	14.596211	37.990775	.65451980+02
45	100.675848	-153.440926	.65340893+02	3	14.596216	157.990749	.65451979+02
16	56.197740	-37.544797	.65395885+02	73	165.403784	118.457194	.65451977+02
17	56.197744	82.455195	.65395885+02	74	165.403788	-121.542809	.65451977+02
18	56.197750	-157.544796	.65395884+02	75	165.403788	-1.542824	.65451977+02
58	123.802253	73.992743	.65395884+02	37	89.999997	-101.776026	.65469022+02
59	123.802254	-46.007258	.65395884+02	38	89.999997	138.223969	.65469020+02
60	123.802258	-166.007254	.65395882+02	39	90.000003	18.223972	.65469021+02
22	64.913403	144.293344	.65397763+02	13	52.611259	112.136600	.65469276+02
23	64.913403	-95.706656	.65397765+02	14	52.611261	-7.863396	.65469277+02
24	64.913404	24.293344	.65397765+02	15	52.611263	-127.863400	.65469277+02
52	115.086591	132.154593	.65397764+02	61	127.388732	-75.688659	.65469276+02
53	115.086593	-107.845396	.65397765+02	62	127.388735	164.311335	.65469275+02
54	115.086599	12.154598	.65397765+02	63	127.388741	44.311344	.65469277+02
10	41.144887	22.994734	.65404679+02	4	29.696553	-17.295695	.65484177+02
11	41.144888	-97.005269	.65404679+02	5	29.696554	102.704292	.65484177+02
12	41.144888	142.994734	.65404678+02	6	29.696554	-137.295694	.65484177+02
64	138.855108	133.453211	.65404677+02	70	150.303440	173.743641	.65484175+02
65	138.855110	-106.546784	.65404678+02	71	150.303440	-66.256351	.65484175+02
66	138.855112	13.453214	.65404678+02	72	150.303446	53.743649	.65484176+02
28	77.620949	-24.850305	.65410738+02	7	37.223231	-58.960400	.65568847+02
29	77.620952	95.149693	.65410738+02	8	37.223236	-178.960384	.65568846+02
30	77.620955	-144.850298	.65410739+02	9	37.223238	61.039598	.65568848+02
46	102.379043	-58.701752	.65410738+02	67	142.776762	95.408340	.65568846+02
47	102.379044	61.298246	.65410739+02	68	142.776764	-24.591657	.65568846+02
48	102.379050	-178.701750	.65410736+02	69	142.776766	-144.591654	.65568845+02
34	82.603442	-76.136075	.65427728+02	25	74.256870	119.999997	.65594990+02
35	82.603446	163.863924	.65427725+02	26	74.256871	-119.999999	.65594992+02
36	82.603449	43.863920	.65427728+02	27	74.256874	.000000	.65594991+02
40	97.396551	112.584020	.65427728+02	49	105.743122	-83.552055	.65594991+02
41	97.396553	-127.415974	.65427728+02	50	105.743124	156.447937	.65594989+02
42	97.396554	-7.415979	.65427727+02	51	105.743132	36.447943	.65594991+02
19	59.909410	-68.025333	.65441767+02	Total Coulomb Energy: 2454.36968904			
20	59.909411	171.974667	.65441765+02				
21	59.909417	51.974662	.65441767+02				

## 76 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
33	83.347381	143.556200	.66265124+02	17	56.799140	69.200486	.66360641+02
34	83.347813	-36.443175	.66265128+02	18	56.799790	-110.799948	.66360653+02
21	60.545635	38.612710	.66305021+02	65	133.455183	160.689724	.66370409+02
22	60.545803	-141.387899	.66305034+02	66	133.455330	-19.310217	.66370406+02
43	96.590390	-79.565669	.66307914+02	23	67.232216	165.098856	.66373847+02
44	96.590731	100.434329	.66307926+02	24	67.232326	-14.900259	.66373838+02
27	72.500681	-90.141873	.66309850+02	73	156.711725	172.543041	.66378737+02
28	72.501293	89.857575	.66309855+02	74	156.711979	-7.458055	.66378736+02
31	77.869253	116.892411	.66315176+02	69	145.994343	-57.033128	.66380120+02
32	77.869588	-63.106957	.66315190+02	70	145.994457	122.967669	.66380122+02
25	70.755392	-168.519064	.66320371+02	61	126.339470	-128.243349	.66382506+02
26	70.755449	11.481767	.66320386+02	62	126.339852	51.756415	.66382504+02
19	60.257660	136.285006	.66328831+02	53	114.086197	178.216019	.66384880+02
20	60.258157	-43.713944	.66328848+02	54	114.086257	-1.783609	.66384879+02
35	85.096879	34.368354	.66336296+02	75	167.858334	-89.304363	.66395018+02
36	85.096993	-145.632341	.66336308+02	76	167.858829	90.697190	.66395016+02
45	100.377524	125.484724	.66343565+02	15	55.047628	107.481036	.66413710+02
46	100.377766	-54.515066	.66343566+02	16	55.047902	-72.517462	.66413743+02
57	120.332294	-75.105903	.66344102+02	37	89.852182	168.673336	.66423536+02
58	120.332619	104.894133	.66344110+02	38	89.852353	-11.326203	.66423532+02
51	111.535283	-151.040434	.66345091+02	13	47.372517	-167.325802	.66440177+02
52	111.535399	28.959645	.66345098+02	14	47.372603	12.674141	.66440178+02
3	21.665006	.000000	.66345276+02	5	33.714037	127.444446	.66440703+02
4	21.665224	-179.999022	.66345277+02	6	33.714075	-52.555662	.66440707+02
8	35.791530	-134.792263	.66351664+02	29	77.561607	58.180344	.66445249+02
7	35.791188	45.206958	.66351679+02	30	77.561836	-121.820459	.66445285+02
49	107.257558	151.973372	.66354182+02	39	92.183167	-103.287497	.66470519+02
50	107.257877	-28.026289	.66354181+02	40	92.184156	76.712431	.66470540+02
63	133.314079	-163.719833	.66357045+02	41	94.278352	12.180048	.66510761+02
64	133.314358	16.280130	.66357052+02	42	94.278419	-167.820459	.66510764+02
55	115.558165	-102.189288	.66357879+02	59	123.382599	132.479462	.66518764+02
56	115.559013	77.810588	.66357901+02	60	123.382783	-47.520517	.66518765+02
67	139.792511	-95.788963	.66358997+02	71	149.518919	-134.756468	.66523619+02
68	139.793194	84.211318	.66359008+02	72	149.519440	45.243296	.66523620+02
47	102.108770	-126.825844	.66359776+02	10	37.002809	-94.445630	.66538332+02
48	102.108885	53.174119	.66359769+02	9	37.001513	85.553967	.66538353+02
2	12.484952	-93.471085	.66360543+02	11	44.525412	-19.578123	.66556501+02
1	12.483901	86.530256	.66360553+02	12	44.525412	160.421875	.66556502+02

Total Coulomb Energy: 2522.67487184



77 POINTS  
D<sub>5</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
37	89.999664	135.174761	.67227488+02	69	140.139612	9.376443	.67312371+02
38	89.999759	63.174767	.67227488+02	7	39.860111	116.973565	.67312381+02
39	90.000051	-152.825222	.67227488+02	8	39.860334	44.973104	.67312375+02
40	90.000193	-8.825216	.67227488+02	9	39.860419	-171.026066	.67312372+02
41	90.000332	-80.825226	.67227488+02	70	140.139664	-134.624363	.67312373+02
32	83.583968	109.745838	.67266247+02	71	140.139858	-62.623928	.67312380+02
33	83.584234	-178.254114	.67266246+02	6	23.658527	-62.152693	.67314159+02
34	83.584244	37.745813	.67266247+02	72	156.341471	116.502092	.67314158+02
35	83.584611	-106.254128	.67266246+02	4	23.658241	9.846580	.67314189+02
36	83.584643	-34.254162	.67266246+02	5	23.658332	-134.151869	.67314179+02
42	96.415321	88.603703	.67266246+02	73	156.341702	44.502920	.67314181+02
43	96.415420	160.603653	.67266246+02	74	156.341745	-171.498653	.67314185+02
44	96.415708	16.603744	.67266247+02	2	23.657848	81.846985	.67314227+02
45	96.415853	-127.396333	.67266247+02	3	23.657907	153.847977	.67314222+02
46	96.415993	-55.396291	.67266248+02	75	156.342104	-27.497351	.67314222+02
22	65.775429	129.701189	.67273521+02	76	156.342123	-99.498270	.67314224+02
23	65.775562	57.701012	.67273520+02	27	73.945366	82.296973	.67337697+02
24	65.775801	-158.298695	.67273517+02	28	73.945421	154.297087	.67337697+02
25	65.776000	-14.298971	.67273516+02	29	73.945771	10.296939	.67337695+02
26	65.776106	-86.298807	.67273514+02	30	73.945849	-133.702879	.67337695+02
52	114.223901	140.648306	.67273515+02	31	73.946031	-61.702979	.67337694+02
53	114.223956	68.648505	.67273516+02	47	106.053942	116.052497	.67337693+02
54	114.224304	-147.351751	.67273518+02	48	106.054182	44.052609	.67337695+02
55	114.224387	-3.351451	.67273519+02	49	106.054238	-171.947582	.67337694+02
56	114.224556	-75.351618	.67273521+02	50	106.054589	-27.947409	.67337697+02
16	48.060164	-65.695002	.67302671+02	51	106.054603	-99.947536	.67337697+02
62	131.939827	120.044494	.67302671+02	17	60.820093	103.549526	.67456696+02
63	131.940039	48.044847	.67302676+02	18	60.820324	175.549742	.67456693+02
12	48.059497	78.304811	.67302686+02	19	60.820405	31.549363	.67456693+02
13	48.059532	150.305208	.67302685+02	20	60.820714	-112.450313	.67456689+02
14	48.059910	6.304685	.67302677+02	21	60.820790	-40.450516	.67456688+02
15	48.059949	-137.694717	.67302677+02	57	119.179182	94.800037	.67456688+02
64	131.940132	-167.955784	.67302677+02	58	119.179320	166.799807	.67456688+02
65	131.940449	-23.955239	.67302684+02	59	119.179547	22.800189	.67456692+02
66	131.940493	-95.955586	.67302686+02	60	119.179757	-121.200161	.67456694+02
10	39.860754	-27.026766	.67312360+02	61	119.179856	-49.199953	.67456696+02
11	39.860785	-99.026266	.67312358+02	1	.000000	-69.998883	.67464465+02
67	140.139206	81.376259	.67312358+02	77	180.000000	113.269457	.67464464+02
68	140.139242	153.375734	.67312359+02				

Total Coulomb Energy: 2591.85015236

## 78 POINTS

 $D_3$ 

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
16	54.961567	148.698465	.68166690+02	52	106.923423	-133.092482	.68237751+02
17	54.961567	-91.301507	.68166692+02	53	106.923424	106.907504	.68237752+02
18	54.961577	28.698469	.68166692+02	54	106.923440	-13.092490	.68237752+02
61	125.038407	152.628796	.68166688+02	19	57.193846	-145.501516	.68242554+02
62	125.038427	-87.371206	.68166691+02	20	57.193847	94.498453	.68242555+02
63	125.038440	32.628795	.68166690+02	21	57.193855	-25.501531	.68242555+02
31	80.041230	143.284712	.68206995+02	58	122.806138	-153.171190	.68242551+02
32	80.041237	-96.715263	.68206997+02	59	122.806143	86.828802	.68242554+02
33	80.041247	23.284719	.68206997+02	60	122.806163	-33.171195	.68242553+02
46	99.958744	158.042549	.68206994+02	34	80.927361	-141.634581	.68254517+02
47	99.958760	-81.957447	.68206997+02	35	80.927363	98.365391	.68254518+02
48	99.958767	38.042540	.68206997+02	36	80.927375	-21.634595	.68254517+02
22	64.022147	121.638389	.68219034+02	43	99.072618	-157.038120	.68254515+02
23	64.022147	-118.361580	.68219034+02	44	99.072627	82.961859	.68254517+02
24	64.022161	1.638401	.68219035+02	45	99.072640	-37.038130	.68254517+02
55	115.977830	179.688873	.68219030+02	28	73.797057	166.496807	.68273979+02
56	115.977849	59.688862	.68219033+02	29	73.797064	-73.503175	.68273982+02
57	115.977851	-60.311132	.68219034+02	30	73.797067	46.496807	.68273982+02
4	30.550313	159.751026	.68222334+02	49	106.202918	134.830458	.68273980+02
5	30.550313	-80.248956	.68222336+02	50	106.202934	-105.169537	.68273982+02
6	30.550319	39.751018	.68222336+02	51	106.202950	14.830453	.68273981+02
73	149.449659	141.576242	.68222331+02	10	40.090614	-118.565271	.68276823+02
74	149.449682	-98.423778	.68222332+02	11	40.090615	121.434706	.68276823+02
75	149.449696	21.576255	.68222333+02	12	40.090626	1.434718	.68276824+02
13	52.843213	179.767908	.68223100+02	67	139.909363	179.892551	.68276818+02
14	52.843216	59.767899	.68223103+02	68	139.909384	59.892569	.68276821+02
15	52.843216	-60.232077	.68223103+02	69	139.909386	-60.107458	.68276821+02
64	127.156765	121.559368	.68223100+02	7	35.362367	82.714779	.68391536+02
65	127.156778	-118.440638	.68223100+02	8	35.362371	-157.285204	.68391535+02
66	127.156799	1.559358	.68223101+02	9	35.362371	-37.285197	.68391536+02
1	13.971519	107.999994	.68232076+02	70	144.637611	98.612500	.68391533+02
2	13.971521	-12.000000	.68232076+02	71	144.637619	-141.387527	.68391532+02
3	13.971521	-132.000002	.68232075+02	72	144.637646	-21.387527	.68391533+02
76	166.028458	-166.672771	.68232070+02	37	87.495112	120.723425	.68401684+02
77	166.028471	73.327358	.68232070+02	38	87.495112	-119.276546	.68401684+02
78	166.028494	-46.672765	.68232070+02	39	87.495128	.723440	.68401685+02
25	73.076556	-165.580225	.68237750+02	40	92.504869	-179.396158	.68401681+02
26	73.076568	74.419748	.68237753+02	41	92.504884	60.603822	.68401685+02
27	73.076575	-45.580234	.68237753+02	42	92.504887	-59.396164	.68401685+02

Total Coulomb Energy: 2662.04721329

## 79 POINTS

 $C_s$ 

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
18	56.045789	-179.999971	.69087725+02	51	109.314930	22.781270	.69182891+02
73	150.956863	-.000315	.69096447+02	52	109.314967	-22.782009	.69182890+02
12	44.809907	-90.000287	.69099712+02	57	113.619664	-101.965985	.69183001+02
13	44.809909	89.999711	.69099718+02	58	113.620226	101.965326	.69183018+02
19	60.221797	-.000381	.69108378+02	26	67.805729	-101.709121	.69183993+02
63	130.353533	124.537570	.69114498+02	27	67.805926	101.708417	.69183986+02
64	130.353539	-124.537626	.69114505+02	39	88.913898	-85.638076	.69185875+02
16	51.916041	-122.390787	.69124398+02	38	88.913647	85.636874	.69185889+02
17	51.916142	122.389926	.69124396+02	79	175.745914	-.000786	.69187066+02
61	123.841418	179.999516	.69127665+02	30	76.990989	-126.567143	.69192895+02
6	27.010399	-120.649784	.69128116+02	31	76.991838	126.565784	.69192899+02
7	27.010681	120.649789	.69128109+02	1	3.287871	179.998890	.69194180+02
14	47.289340	54.910401	.69134959+02	53	110.394931	-47.940900	.69201845+02
15	47.289515	-54.911236	.69134960+02	54	110.395110	47.940150	.69201845+02
74	154.287666	-55.639010	.69141206+02	42	91.219612	-62.139817	.69204552+02
75	154.287691	55.638286	.69141206+02	43	91.219697	62.138784	.69204556+02
76	155.206236	-115.352504	.69154048+02	62	126.002438	-.000239	.69210233+02
77	155.206409	115.352300	.69154055+02	69	135.729742	-91.661340	.69223910+02
8	40.753477	-20.684664	.69157501+02	70	135.730108	91.660958	.69223918+02
9	40.753520	20.683909	.69157505+02	20	63.396180	-27.667406	.69225880+02
67	133.208702	-29.317974	.69158884+02	21	63.396223	27.666653	.69225880+02
68	133.208731	29.317533	.69158879+02	22	65.710076	-148.240992	.69245908+02
24	66.566330	75.975119	.69163021+02	23	65.710091	148.238876	.69245944+02
25	66.566597	-75.975907	.69163013+02	33	78.219034	-168.321627	.69257541+02
50	105.604944	127.346813	.69166392+02	32	78.217822	168.320059	.69257554+02
49	105.604769	-127.347476	.69166406+02	46	101.474730	168.319878	.69270147+02
55	111.314815	76.613428	.69167770+02	47	101.475732	-168.319929	.69270193+02
56	111.314908	-76.613995	.69167780+02	11	43.487739	153.610968	.69280104+02
40	91.173519	-146.186234	.69168288+02	10	43.487289	-153.611029	.69280126+02
41	91.173723	146.185608	.69168290+02	5	26.143251	179.999454	.69288207+02
71	140.463453	156.848316	.69169762+02	44	91.240651	-108.383994	.69323794+02
72	140.463459	-156.848938	.69169760+02	45	91.241298	108.382556	.69323796+02
34	82.422830	-12.736498	.69170617+02	48	102.037570	-.000392	.69330988+02
35	82.422833	12.735707	.69170618+02	78	160.966103	-179.999962	.69334899+02
36	88.899985	35.682181	.69171988+02	28	70.698117	51.439291	.69337278+02
37	88.899987	-35.682954	.69171989+02	29	70.698205	-51.440009	.69337282+02
59	117.245677	150.040264	.69177642+02	65	130.768244	60.671643	.69337658+02
60	117.246080	-150.040270	.69177682+02	66	130.768272	-60.671943	.69337663+02
3	24.474598	64.171263	.69180023+02	2	19.955384	.000001	.69358494+02
4	24.474663	-64.171197	.69180025+02				

Total Coulomb Energy: 2733.24835748

## 80 POINTS

 $D_{4d} (S_{8v})$ 

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
21	63.775159	- .000000	.70065550+02	13	53.318625	-26.290715	.70130985+02
22	63.775156	-90.000000	.70065550+02	14	53.318624	-63.709284	.70130985+02
23	63.775159	89.999998	.70065550+02	15	53.318627	26.290715	.70130985+02
24	63.775155	179.999998	.70065550+02	16	53.318627	63.709283	.70130985+02
57	116.224843	-45.000002	.70065550+02	17	53.318622	-116.290716	.70130985+02
58	116.224846	44.999999	.70065550+02	18	53.318622	-153.709286	.70130985+02
59	116.224840	-135.000002	.70065550+02	19	53.318625	116.290712	.70130985+02
60	116.224843	135.000000	.70065550+02	20	53.318624	153.709282	.70130985+02
5	33.588264	-44.999997	.70083202+02	61	126.681377	-18.709287	.70130985+02
6	33.588266	44.999999	.70083202+02	62	126.681378	18.709283	.70130985+02
7	33.588261	-135.000002	.70083202+02	63	126.681375	-71.290718	.70130985+02
8	33.588263	134.999994	.70083202+02	64	126.681374	-108.709287	.70130985+02
73	146.411739	- .000004	.70083202+02	65	126.681378	71.290715	.70130985+02
74	146.411736	-90.000004	.70083202+02	66	126.681376	108.709286	.70130985+02
75	146.411739	90.000002	.70083202+02	67	126.681374	-161.290716	.70130985+02
76	146.411736	-179.999998	.70083202+02	68	126.681375	161.290716	.70130985+02
29	78.135483	-21.850208	.70085566+02	9	39.077461	.000001	.70146818+02
30	78.135484	21.850207	.70085566+02	10	39.077458	-89.999999	.70146818+02
31	78.135481	-68.149793	.70085566+02	11	39.077461	89.999996	.70146818+02
32	78.135479	-111.850208	.70085566+02	12	39.077457	179.999996	.70146818+02
33	78.135484	68.149791	.70085566+02	69	140.922541	-45.000004	.70146818+02
34	78.135483	111.850206	.70085566+02	70	140.922543	44.999999	.70146818+02
35	78.135479	-158.149794	.70085566+02	71	140.922539	-135.000002	.70146818+02
36	78.135481	158.149792	.70085566+02	72	140.922541	135.000002	.70146818+02
45	101.864520	-23.149794	.70085566+02	1	16.299099	.000005	.70228641+02
46	101.864518	-66.850209	.70085566+02	2	16.299095	-89.999994	.70228641+02
47	101.864521	23.149791	.70085566+02	3	16.299099	89.999992	.70228641+02
48	101.864521	66.850206	.70085566+02	4	16.299095	179.999992	.70228641+02
49	101.864516	-113.149794	.70085566+02	77	163.700903	-45.000010	.70228641+02
50	101.864516	-156.850208	.70085566+02	78	163.700907	45.000000	.70228641+02
51	101.864519	113.149792	.70085566+02	79	163.700901	-135.000002	.70228641+02
52	101.864517	156.850206	.70085566+02	80	163.700903	135.000008	.70228641+02
37	87.828323	- .000001	.70125118+02	25	69.359200	-45.000000	.70256536+02
38	87.828320	-90.000001	.70125118+02	26	69.359203	44.999999	.70256536+02
39	87.828323	89.999999	.70125118+02	27	69.359198	-135.000002	.70256536+02
40	87.828320	179.999998	.70125119+02	28	69.359200	134.999998	.70256536+02
41	92.171679	-45.000001	.70125118+02	53	110.640801	- .000002	.70256536+02
42	92.171681	44.999999	.70125118+02	54	110.640798	-90.000002	.70256536+02
43	92.171676	-135.000002	.70125118+02	55	110.640801	90.000000	.70256536+02
44	92.171679	135.000000	.70125119+02	56	110.640798	180.000000	.70256536+02

Total Coulomb Energy: 2805.35587598

81 POINTS  
C<sub>2</sub> (MIN ENERGY)

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
17	51.484429	-58.571881	.70979072+02	75	147.257587	-51.971842	.71049395+02
16	51.484115	121.427712	.70979102+02	12	43.566561	152.678762	.71050099+02
32	77.571155	-61.272240	.70989731+02	13	43.568825	-27.320461	.71050093+02
33	77.571235	118.728858	.70989783+02	38	86.715482	-150.538967	.71059374+02
80	167.458609	88.801281	.70991083+02	39	86.718092	29.460696	.71059367+02
81	167.459181	-91.208000	.70991086+02	56	112.736322	-88.381840	.71060708+02
27	67.907395	-38.543052	.70995517+02	57	112.736520	91.618965	.71060706+02
26	67.905901	141.457684	.70995530+02	1	.002542	51.983070	.71077717+02
43	92.331699	-41.780719	.70998130+02	14	47.581749	-170.992601	.71078021+02
42	92.330509	138.220564	.70998153+02	15	47.585028	9.004761	.71078084+02
68	134.121540	158.031021	.71010139+02	60	117.757839	136.902006	.71089986+02
69	134.123768	-21.969994	.71010143+02	61	117.759548	-43.099533	.71089992+02
44	93.420479	-176.917006	.71015597+02	28	71.973028	-169.361099	.71097626+02
45	93.423080	3.082244	.71015597+02	29	71.975942	10.638005	.71097629+02
4	24.186726	-178.716770	.71017605+02	24	64.612361	-81.977947	.71100058+02
5	24.189067	1.285174	.71017595+02	25	64.614075	98.023019	.71100151+02
78	159.113173	176.242798	.71024165+02	77	148.144909	49.729149	.71100555+02
79	159.115257	-3.756355	.71024156+02	76	148.143951	-130.273958	.71100566+02
48	102.104651	116.318889	.71024554+02	36	84.549707	161.334770	.71115532+02
49	102.105402	-63.681849	.71024558+02	37	84.552540	-18.666346	.71115557+02
35	79.688905	53.081652	.71029176+02	55	108.561953	22.962375	.71133867+02
34	79.687709	-126.918222	.71029202+02	54	108.559547	-157.037476	.71133878+02
19	56.139579	63.676958	.71029218+02	71	137.412710	12.976669	.71142862+02
18	56.139425	-116.320316	.71029235+02	70	137.410765	-167.024094	.71142876+02
40	89.383760	-83.573631	.71032692+02	52	107.093102	158.546652	.71150559+02
41	89.384154	96.426134	.71032684+02	53	107.095527	-21.454651	.71150577+02
62	122.528640	-112.477648	.71033544+02	30	75.565007	76.750891	.71160510+02
63	122.528728	67.523515	.71033538+02	31	75.566042	-103.248673	.71160586+02
46	98.289557	71.878171	.71033916+02	8	40.341101	-139.006563	.71175509+02
47	98.289873	-108.122342	.71033973+02	9	40.343993	40.987797	.71175608+02
10	42.983265	-91.144690	.71036457+02	64	125.607038	-139.832731	.71181841+02
11	42.986211	88.854312	.71036498+02	65	125.608457	40.168482	.71181848+02
51	102.992553	48.552930	.71039110+02	66	126.368980	112.560176	.71185255+02
50	102.991349	-131.447540	.71039132+02	67	126.370010	-67.441819	.71185259+02
6	26.800472	123.585608	.71045424+02	3	22.841605	67.185228	.71209045+02
7	26.800810	-56.408287	.71045446+02	2	22.836419	-112.810874	.71209079+02
20	63.083173	-145.033653	.71048688+02	22	63.252869	167.468964	.71209145+02
21	63.086184	34.964769	.71048726+02	23	63.256190	-12.532084	.71209170+02
72	140.839039	87.311879	.71048842+02	58	117.207576	-179.999161	.71210954+02
73	140.839493	-92.690742	.71048868+02	59	117.209870	.000134	.71210963+02
74	147.255978	128.030672	.71049389+02				

Total Coulomb Energy: 2878.52282967

81 POINTS  
C<sub>2</sub> (NON-MINIMUM ENERGY)

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
21	63.991799	162.865549	.70929919+02	65	127.215482	-38.573100	.71056602+02
22	63.996710	-17.127875	.70929954+02	66	127.216920	141.440506	.71056600+02
49	102.544249	-40.262258	.70964099+02	1	11.998812	169.062880	.71061558+02
50	102.546134	139.740223	.70964112+02	2	12.004465	-10.850400	.71061581+02
53	110.815083	-113.287277	.70978657+02	55	112.816912	162.612362	.71065855+02
54	110.833252	66.715180	.70978662+02	56	112.823289	-17.393882	.71065860+02
43	92.121504	-130.846310	.70993074+02	14	46.596069	101.314604	.71066110+02
44	92.141066	49.153005	.70993090+02	13	46.582654	-78.669901	.71066128+02
59	114.516484	-63.772534	.70998549+02	70	135.010664	59.458748	.71068359+02
60	114.525816	116.234431	.70998554+02	69	134.991364	-120.546548	.71068378+02
33	77.374646	-41.852860	.71001072+02	3	21.931874	-101.433968	.71072383+02
34	77.377454	138.141621	.71001128+02	4	21.949733	78.550523	.71072375+02
71	136.662167	171.281742	.71012632+02	11	44.295227	-112.708032	.71080606+02
72	136.671631	-8.735874	.71012624+02	12	44.313181	67.284202	.71080638+02
39	88.538499	-106.370918	.71019976+02	8	31.459951	27.674747	.71084375+02
40	88.555634	73.628111	.71019979+02	7	31.443399	-152.338827	.71084423+02
38	87.164977	-20.884218	.71023434+02	23	64.474310	-97.320818	.71089266+02
37	87.159903	159.113144	.71023496+02	24	64.490032	82.671049	.71089334+02
75	154.688190	-97.158379	.71025949+02	32	75.688340	5.812115	.71096216+02
76	154.705816	82.861091	.71025955+02	31	75.675464	-174.188904	.71096245+02
52	104.527759	93.179378	.71032121+02	64	126.736216	87.839939	.71114452+02
51	104.515755	-86.823879	.71032150+02	63	126.722368	-92.169710	.71114471+02
30	75.061549	30.832798	.71035858+02	19	53.937084	-169.563276	.71136932+02
29	75.043261	-149.166355	.71035891+02	20	53.950961	10.444343	.71136940+02
17	53.740004	-42.187562	.71037084+02	79	156.798237	-156.022270	.71145690+02
18	53.743615	137.801184	.71037107+02	80	156.816366	23.953523	.71145732+02
42	91.507543	118.444856	.71038386+02	62	117.110492	10.395200	.71150542+02
41	91.499540	-61.553579	.71038427+02	61	117.094476	-169.599703	.71150553+02
57	114.356474	-139.078148	.71039590+02	36	82.223974	97.175484	.71183252+02
58	114.376501	40.921227	.71039600+02	35	82.213650	-82.821874	.71183271+02
78	154.969301	143.996553	.71043961+02	6	31.342077	128.080515	.71203854+02
77	154.969023	-36.046668	.71043987+02	5	31.333944	-51.889373	.71203910+02
25	66.536646	-65.110083	.71045406+02	74	138.252863	114.093548	.71208706+02
26	66.544370	114.883292	.71045407+02	73	138.242121	-65.924117	.71208729+02
81	179.989653	-126.673086	.71048585+02	15	53.539215	-140.662575	.71221255+02
27	70.148246	-122.236239	.71051242+02	16	53.558160	39.338141	.71221263+02
28	70.167630	57.760077	.71051272+02	68	134.840654	27.017878	.71264959+02
47	96.784255	-155.666422	.71054622+02	67	134.821486	-152.976280	.71264985+02
48	96.802196	24.333287	.71054665+02	45	96.550842	179.996447	.71267673+02
9	38.964388	166.304731	.71054834+02	46	96.563665	-.003217	.71267669+02
10	38.970624	-13.673965	.71054854+02				

Total Coulomb Energy: 2878.54384730

## 82 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
25	65.923039	144.583750	.71888980+02	58	111.405357	-54.934021	.71986575+02
26	65.923183	-35.416817	.71888979+02	49	103.153510	61.218113	.71997408+02
33	79.060518	65.826031	.71897722+02	50	103.154807	-118.781860	.71997408+02
34	79.061803	-114.173954	.71897723+02	1	11.876062	53.632961	.72005840+02
41	89.176445	133.769575	.71917789+02	2	11.877356	-126.366354	.72005840+02
42	89.176839	-46.230446	.71917789+02	3	22.005782	135.622810	.72009215+02
69	132.471186	136.962061	.71927834+02	4	22.006117	-44.380304	.72009214+02
70	132.471527	-43.036800	.71927834+02	73	143.934582	25.315414	.72011263+02
55	109.183763	149.638535	.71928527+02	74	143.935627	-154.687656	.72011263+02
56	109.183814	-30.361024	.71928528+02	13	45.714422	126.523973	.72014387+02
39	86.181718	-23.083925	.71944999+02	14	45.714955	-53.477146	.72014387+02
40	86.181836	156.916180	.71944999+02	45	97.001921	83.471020	.72026497+02
61	121.991377	15.864060	.71946400+02	46	97.003108	-96.528896	.72026497+02
62	121.992280	-164.136509	.71946400+02	79	157.755951	116.484287	.72028176+02
21	61.989279	44.661839	.71949224+02	80	157.756710	-63.513117	.72028176+02
22	61.990522	-135.337938	.71949224+02	51	105.485602	-5.569470	.72030280+02
43	90.820559	109.298182	.71952060+02	52	105.486094	174.430210	.72030279+02
44	90.821436	-70.701794	.71952060+02	29	73.751236	21.916207	.72039806+02
9	38.535525	48.607137	.71957293+02	30	73.752255	-158.083511	.72039806+02
10	38.536793	-131.392529	.71957293+02	23	63.053758	-8.180355	.72043023+02
15	51.753473	16.845958	.71959119+02	24	63.054213	171.820257	.72043024+02
16	51.754426	-163.153328	.71959118+02	65	127.572407	-11.844691	.72051588+02
81	168.254143	32.973423	.71963248+02	66	127.572768	168.154364	.72051587+02
82	168.255281	-147.029625	.71963248+02	67	127.877990	49.354287	.72086749+02
27	69.938110	119.316605	.71968213+02	68	127.879265	-130.645929	.72086749+02
28	69.938791	-60.683786	.71968212+02	47	97.411335	18.202367	.72099606+02
71	135.152920	105.130476	.71972445+02	48	97.412288	-161.797733	.72099606+02
72	135.153873	-74.868635	.71972445+02	11	43.724231	-21.059819	.72107387+02
7	32.908888	88.134249	.71975570+02	12	43.724417	158.941492	.72107387+02
8	32.910030	-91.866681	.71975570+02	59	112.617906	100.874925	.72135107+02
75	146.902998	70.056480	.71976254+02	60	112.618918	-79.124735	.72135107+02
76	146.904287	-109.943240	.71976255+02	77	149.679968	-15.373799	.72139110+02
37	85.563507	42.895097	.71976296+02	78	149.680254	164.624022	.72139109+02
38	85.564743	-137.104830	.71976297+02	5	29.655045	9.612536	.72148183+02
63	122.494156	77.032894	.71976810+02	6	29.655884	-170.385700	.72148182+02
64	122.495408	-102.966887	.71976810+02	17	54.617085	99.291578	.72162578+02
19	56.279216	71.266323	.71979578+02	18	54.618080	-80.708962	.72162579+02
20	56.280480	-108.733805	.71979578+02	53	108.339581	37.886633	.72199322+02
31	75.576591	90.825194	.71985916+02	54	108.340765	-142.113516	.72199321+02
32	75.577700	-89.174937	.71985915+02	35	83.089257	- .001754	.72208411+02
57	111.404769	125.065526	.71986575+02	36	83.089862	179.998413	.72208411+02

Total Coulomb Energy: 2952.57478472

## 83 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
79	88.556324	-147.687544	.72847680+02	62	63.709200	31.679684	.72937522+02
8	88.556282	32.312032	.72847790+02	47	63.713737	-148.095043	.72937929+02
48	49.181745	55.326939	.72862772+02	32	25.504151	-121.338305	.72943065+02
27	49.356187	-124.326190	.72862916+02	52	25.309345	57.851353	.72943118+02
77	89.342925	-103.772778	.72875329+02	74	103.047235	161.602295	.72943353+02
38	89.040468	76.229265	.72875416+02	53	103.382992	-18.342069	.72943721+02
83	146.127539	-9.251653	.72877391+02	22	41.845335	87.814470	.72957212+02
66	145.842583	170.274166	.72877484+02	33	42.202573	-91.912342	.72957326+02
54	57.479612	-.989030	.72879495+02	78	157.118658	36.675884	.72967733+02
51	57.233135	179.227974	.72879642+02	59	157.153112	-144.337173	.72967813+02
70	121.629226	179.071369	.72881701+02	26	126.189344	151.248661	.72969410+02
71	121.869262	-.707085	.72881829+02	37	126.562376	-28.603556	.72969405+02
3	65.468477	77.245246	.72889294+02	20	135.822523	60.121235	.72970825+02
12	65.773286	-102.607982	.72889373+02	67	136.027384	-120.270337	.72971038+02
82	134.329540	24.774701	.72891330+02	55	85.533125	144.089464	.72971832+02
50	134.276594	-155.645315	.72891462+02	81	85.930494	-35.920677	.72971947+02
24	106.040187	-83.847342	.72893693+02	34	.213177	-59.701176	.72977862+02
30	105.657329	96.209572	.72893829+02	9	82.950099	-81.597226	.72979880+02
6	79.046268	167.443909	.72894805+02	42	82.561970	98.386380	.72980095+02
21	79.352129	-12.611387	.72894939+02	19	129.609379	-87.841851	.72980495+02
61	24.321394	118.184266	.72895308+02	36	129.238880	92.337420	.72980489+02
1	24.752664	-61.757389	.72895387+02	69	109.604442	22.898238	.72993063+02
35	42.378788	22.195635	.72898411+02	58	109.537787	-157.252789	.72993192+02
18	42.318108	-157.332277	.72898436+02	4	97.215121	-176.044682	.73016963+02
10	142.412445	128.456728	.72901842+02	25	97.429902	3.995381	.73017553+02
23	142.836861	-51.481735	.72901921+02	16	76.506757	-167.744934	.73022972+02
40	95.113887	-61.815860	.72906670+02	46	76.673661	12.164823	.73023072+02
2	94.691833	118.193065	.72906778+02	17	95.961537	-126.036944	.73027741+02
76	168.496662	-38.568269	.72907582+02	64	95.797573	54.016852	.73027939+02
11	168.090754	140.746414	.72907641+02	56	41.248743	-22.139214	.73032194+02
29	113.079364	-107.918058	.72908088+02	49	40.898112	158.124229	.73032698+02
80	112.803266	72.225065	.72908078+02	68	116.463408	45.614159	.73055280+02
72	72.354673	124.786043	.72908778+02	28	116.569783	-134.595573	.73055591+02
73	72.782050	-55.213399	.72908865+02	45	151.940493	90.030390	.73104802+02
5	120.390229	117.799895	.72918127+02	43	152.303587	-90.395535	.73104855+02
57	120.816224	-62.225465	.72918136+02	41	107.604446	-42.394208	.73109113+02
13	73.404174	54.141262	.72920618+02	75	107.194047	137.580227	.73109146+02
7	73.571236	-125.730751	.72920742+02	44	61.376609	-76.850595	.73113584+02
39	63.064003	-30.672972	.72922542+02	63	60.974341	103.057968	.73113750+02
31	62.683305	149.418213	.72922635+02	65	22.527084	-179.103491	.73128573+02
60	47.738965	-54.263173	.72929515+02	15	22.738098	.000388	.73128766+02
14	47.314240	125.743702	.72929794+02				

Total Coulomb Energy: 3027.52848897



## 84 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
37	179.999998	164.341694	.73782935+02	29	62.289464	-36.507625	.73877988+02
13	87.351216	-99.527990	.73807408+02	78	62.289135	143.492296	.73877991+02
64	87.351224	80.472007	.73807408+02	11	48.842395	-9.435743	.73878822+02
43	135.610096	-17.390289	.73808107+02	71	48.842044	170.564255	.73878828+02
59	135.609772	162.609758	.73808097+02	25	114.399078	-4.459533	.73878927+02
15	92.406394	104.062654	.73811769+02	66	114.398753	175.540449	.73878921+02
50	92.406538	-75.937366	.73811770+02	54	104.525163	-115.974425	.73884140+02
69	.000000	-11.235151	.73814801+02	70	104.525266	64.025677	.73884141+02
44	43.969861	89.170283	.73817576+02	68	89.170829	-175.474049	.73889168+02
76	43.969923	-90.829360	.73817573+02	83	89.171158	4.525957	.73889171+02
28	43.122967	-157.172005	.73824672+02	53	23.938514	-70.080842	.73900617+02
61	43.123264	22.827800	.73824665+02	51	23.938324	109.918444	.73900636+02
16	156.208183	-172.829945	.73828263+02	14	53.676412	-63.686014	.73903824+02
82	156.208496	7.170268	.73828294+02	48	53.676194	116.313782	.73903827+02
27	113.209715	148.292097	.73830123+02	10	24.416120	53.251829	.73905898+02
33	113.210027	-31.707951	.73830127+02	21	24.415963	-126.747451	.73905911+02
12	76.794186	-58.482957	.73833659+02	60	110.457664	87.363554	.73910920+02
35	76.793946	121.516984	.73833659+02	65	110.457696	-92.636589	.73910921+02
67	136.796595	98.538816	.73839562+02	47	130.264435	-48.818273	.73912060+02
81	136.796726	-81.461546	.73839566+02	80	130.264179	131.181917	.73912054+02
20	107.465853	19.501049	.73840581+02	32	64.436753	73.132045	.73917935+02
46	107.465566	-160.499004	.73840577+02	74	64.436712	-106.867795	.73917935+02
3	24.013289	-4.960408	.73844667+02	31	119.899099	42.295040	.73922696+02
26	24.012931	175.039682	.73844701+02	39	119.898896	-137.705118	.73922693+02
22	69.547613	-82.733708	.73845438+02	4	157.154654	77.601749	.73924995+02
30	69.547506	97.266171	.73845438+02	45	157.154676	-102.399044	.73924998+02
18	80.295334	56.669835	.73847566+02	8	84.999138	143.729750	.73961599+02
79	80.295191	-123.330128	.73847565+02	57	84.999471	-36.270248	.73961599+02
23	64.105261	39.507511	.73848898+02	41	46.743446	56.394548	.73982089+02
55	64.105033	-140.492378	.73848900+02	52	46.743310	-123.605161	.73982090+02
6	72.058750	-13.249138	.73849336+02	38	115.692428	-69.268641	.74001068+02
17	72.058410	166.750854	.73849336+02	58	115.692233	110.731535	.74001065+02
19	64.807405	11.295334	.73857923+02	7	82.621385	26.288043	.74008032+02
73	64.807082	-168.704613	.73857925+02	34	82.621108	-153.711943	.74008032+02
2	100.835926	-52.159814	.73862531+02	72	39.446952	-39.457671	.74034463+02
9	100.835649	127.840248	.73862530+02	1	39.446624	140.542116	.74034473+02
40	153.500830	132.787247	.73864471+02	63	95.393868	-17.068902	.74049996+02
49	153.501091	-47.213151	.73864494+02	75	95.393539	162.931095	.74049993+02
56	131.309963	14.765818	.73868100+02	5	142.522539	44.523887	.74054421+02
77	131.309671	-165.234293	.73868091+02	62	142.522348	-135.476433	.74054413+02
24	128.183136	70.184451	.73873268+02	42	97.362093	-138.000050	.74062632+02
36	128.183069	-109.815806	.73873268+02	84	97.362302	42.000000	.74062633+02

Total Coulomb Energy: 3103.46512443

## 85 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
41	89.909480	-150.313438	.74711785+02	11	42.348286	-122.975564	.74819928+02
42	89.909634	29.686560	.74711781+02	12	42.583614	57.517458	.74819931+02
33	75.461593	-12.183308	.74736540+02	68	126.211637	65.933746	.74822602+02
34	75.802464	167.720375	.74736541+02	67	125.909575	-113.767213	.74822641+02
54	106.963554	138.401426	.74747844+02	80	149.834492	65.632002	.74825180+02
53	106.481448	-41.647092	.74747857+02	79	149.532904	-113.667505	.74825228+02
55	109.011879	-132.235285	.74762258+02	70	131.633806	129.600000	.74833673+02
56	109.169171	47.596644	.74762251+02	69	131.132866	-50.382144	.74833703+02
21	58.608109	-31.543908	.74773568+02	49	98.01550	-18.140000	.748337157+02
22	59.055277	148.309151	.74773566+02	50	98.393053	161.908745	.748337149+02
85	179.746950	-60.046701	.74774740+02	75	136.478218	-81.248413	.74837838+02
13	46.989503	26.120053	.74774940+02	76	136.951439	98.556357	.74837871+02
14	47.023539	-154.353577	.74774939+02	31	72.255259	-77.926784	.74838508+02
1	11.913360	-45.262439	.74779016+02	32	72.740140	102.121842	.74838514+02
2	12.406477	134.138859	.74779020+02	17	52.839304	-5.310887	.74841057+02
45	91.136176	-173.505253	.74779047+02	18	53.133423	174.376091	.74841065+02
43	90.934766	6.485793	.74779067+02	47	94.235170	-83.378384	.74843183+02
72	133.079422	37.713346	.74783456+02	48	94.702679	96.605776	.74843198+02
71	133.006020	-141.815598	.74783494+02	65	122.202191	-23.186937	.74845781+02
9	36.388631	-39.599083	.74785611+02	66	122.607245	157.008198	.74845800+02
10	36.866138	140.160288	.74785615+02	25	67.673648	-143.191067	.74853998+02
82	157.524019	-160.543953	.74788359+02	26	67.737783	37.015154	.74854007+02
81	157.426657	18.250613	.74788435+02	62	113.491304	114.059603	.74865612+02
39	86.401982	-127.025197	.74791142+02	61	112.985067	-65.918183	.74865646+02
40	86.603053	53.002462	.74791150+02	73	134.013218	7.077708	.74866858+02
36	79.696548	78.550190	.74791794+02	74	134.207714	-172.464413	.74866868+02
35	79.313847	-101.511429	.74791818+02	3	20.600562	-134.718027	.74870832+02
29	69.601663	-167.277397	.74792605+02	4	20.742319	46.579471	.74870855+02
27	69.453069	12.903668	.74792622+02	15	50.118028	-65.478023	.74911293+02
7	31.289641	-85.436398	.74804286+02	16	50.625350	114.559763	.74911312+02
8	31.751400	94.914660	.74804301+02	24	64.728661	60.926636	.74938518+02
51	100.945408	-109.068816	.74806043+02	23	64.465743	-119.279455	.74938541+02
52	101.279986	70.854897	.74806060+02	77	145.603165	-23.666744	.74940043+02
19	54.609180	-94.877556	.74806573+02	78	146.009464	156.784662	.74940070+02
20	55.028852	85.325088	.74806570+02	5	30.872520	-3.302114	.74946995+02
38	83.885008	144.646971	.74808112+02	6	31.130687	178.965944	.74946993+02
37	83.423202	-35.329478	.74808124+02	30	69.959829	126.534606	.74996976+02
46	91.450082	120.181684	.74813657+02	28	69.454431	-53.443512	.74996996+02
44	90.941287	-59.818311	.74813669+02	63	115.468797	-90.697971	.74999726+02
57	112.059316	23.939952	.74814025+02	64	115.906084	89.176607	.74999747+02
58	112.109118	-155.854147	.74814024+02	60	112.603168	-179.816689	.74999952+02
83	157.765835	-63.556651	.74815174+02	59	112.350720	.000000	.74999972+02
84	158.270819	116.373280	.74815226+02				

Total Coulomb Energy: 3180.38926265

## 86 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
7	35.191968	-101.297685	.75650486+02	44	86.997127	169.191599	.75760832+02
8	35.240026	78.715513	.75650486+02	13	43.644400	-66.901854	.75763039+02
33	78.681264	-107.333440	.75658953+02	14	43.689316	113.077786	.75763039+02
34	78.728064	72.669417	.75658954+02	45	95.239305	-169.076918	.75763507+02
17	56.104057	-121.400054	.75665125+02	46	95.248835	10.918663	.75763508+02
18	56.145986	58.616912	.75665125+02	53	102.616677	-72.571325	.75767777+02
49	99.356393	-120.240973	.75666184+02	54	102.663272	107.432031	.75767778+02
50	99.398815	59.754999	.75666185+02	47	99.076169	-143.942474	.75781493+02
85	167.972097	-79.752769	.75671879+02	48	99.105201	36.051226	.75781493+02
86	168.020195	100.289418	.75671879+02	41	84.125057	-58.435480	.75781945+02
83	159.925991	-167.285458	.75677362+02	42	84.166620	121.561892	.75781945+02
84	159.936960	12.584005	.75677362+02	61	117.094468	-160.628843	.75786029+02
81	148.449236	-36.292829	.75694913+02	62	117.110928	19.347568	.75786030+02
82	148.477978	143.771704	.75694912+02	59	112.547542	-5.125501	.75786493+02
25	64.283397	-18.964160	.75702270+02	60	112.551649	174.894760	.75786492+02
26	64.299067	161.013523	.75702270+02	71	126.257882	-56.789938	.75788949+02
21	58.265768	-95.100245	.75703381+02	72	126.298695	123.229918	.75788948+02
22	58.314543	84.902288	.75703381+02	23	62.093345	-45.958299	.75792473+02
51	102.128257	-97.973417	.75703557+02	24	62.128350	134.023615	.75792473+02
52	102.176744	82.025190	.75703558+02	57	104.970073	-49.031720	.75804008+02
31	77.658171	-130.114599	.75709118+02	58	105.006866	130.976929	.75804008+02
32	77.695784	49.892239	.75709119+02	69	125.560491	-29.355770	.75811564+02
79	146.642513	-116.136315	.75733536+02	70	125.584253	150.674856	.75811563+02
80	146.686535	63.831223	.75733535+02	77	144.415504	-77.626294	.75812370+02
73	136.118492	-2.380924	.75741240+02	78	144.463242	102.388703	.75812369+02
74	136.120258	177.669950	.75741239+02	3	22.082338	-55.884092	.75815210+02
9	35.889704	-140.199091	.75745583+02	4	22.122725	124.047811	.75815210+02
10	35.921271	39.852587	.75745583+02	29	70.838592	-174.462511	.75824840+02
11	42.922063	-30.803288	.75749773+02	30	70.843583	5.554403	.75824841+02
12	42.946914	149.151392	.75749773+02	63	119.514042	-133.657953	.75854312+02
15	48.666738	-176.410452	.75749773+02	64	119.549644	46.323022	.75854311+02
16	48.670089	3.632498	.75749773+02	65	122.105645	-83.759234	.75881470+02
19	57.237393	-149.151138	.75754408+02	66	122.154245	96.244301	.75881470+02
20	57.262744	30.875800	.75754408+02	75	138.482058	-149.432537	.75885143+02
1	11.664991	-128.202957	.75755816+02	76	138.507147	30.519947	.75885143+02
2	11.703675	51.942151	.75755817+02	5	26.971887	-1.219838	.75925039+02
67	124.074086	-109.308963	.75757089+02	6	26.972697	178.683990	.75925038+02
68	124.120338	70.680278	.75757089+02	27	65.544950	-71.313419	.75934050+02
39	83.213995	-84.979954	.75758309+02	28	65.591226	108.679365	.75934050+02
40	83.262708	95.019514	.75758310+02	35	78.881001	-152.882954	.75944894+02
37	82.351895	-35.095768	.75759747+02	36	78.903566	27.125570	.75944895+02
38	82.379829	144.898861	.75759747+02	55	103.145967	-26.485783	.75946019+02
43	86.988198	-10.805885	.75760833+02	56	103.167563	153.524490	.75946019+02

Total Coulomb Energy: 3258.21995933

## 87 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
71	132.716690	55.501344	.76591058+02	57	110.236865	54.788148	.76706185+02
72	132.717924	-124.497934	.76591058+02	58	110.238103	-125.211580	.76706185+02
7	32.879108	8.870615	.76592431+02	67	119.623003	80.118412	.76706623+02
8	32.880498	-171.128849	.76592431+02	68	119.623798	-99.880904	.76706623+02
1	12.362654	-33.826479	.76608274+02	33	77.011713	-.004704	.76706694+02
2	12.363442	146.178965	.76608274+02	34	77.013033	179.995428	.76706694+02
51	98.055131	-9.889776	.76608970+02	41	84.125944	57.951218	.76706881+02
52	98.056337	170.110128	.76608970+02	42	84.127123	-122.048876	.76706881+02
69	120.717053	3.008059	.76613184+02	13	44.213465	41.565493	.76708190+02
70	120.718418	-176.992224	.76613184+02	14	44.214822	-138.434984	.76708190+02
63	116.817640	30.562561	.76635805+02	17	54.535969	-8.607004	.76710999+02
64	116.819085	-149.437342	.76635806+02	18	54.537188	171.393536	.76710999+02
3	19.276687	54.235341	.76637615+02	47	96.327515	-60.267170	.76716876+02
4	19.277905	-125.766798	.76637616+02	48	96.327701	119.732695	.76716876+02
29	76.207209	107.449950	.76638402+02	73	136.041000	-51.157212	.76716920+02
30	76.207337	-72.550422	.76638402+02	74	136.041420	128.841339	.76716920+02
55	100.173525	13.022307	.76640225+02	25	61.779280	65.551903	.76719084+02
56	100.174951	-166.977732	.76640225+02	26	61.780332	-114.448633	.76719084+02
65	118.823023	106.797706	.76641039+02	61	116.636690	-23.025052	.76734350+02
66	118.823173	-73.201517	.76641039+02	62	116.637692	156.974449	.76734351+02
75	138.139635	22.897941	.76659663+02	35	77.330997	-22.537130	.76738043+02
76	138.141096	-157.102058	.76659663+02	36	77.332011	157.463104	.76738043+02
49	98.034491	97.134496	.76672593+02	27	67.860993	41.590662	.76747504+02
50	98.034882	-82.865329	.76672593+02	28	67.862355	-138.409531	.76747505+02
77	138.224634	-17.736701	.76675595+02	21	56.889597	17.376761	.76750341+02
78	138.225731	162.262234	.76675595+02	22	56.891029	-162.623144	.76750342+02
5	32.195819	109.190792	.76679126+02	19	56.749506	93.135758	.76777051+02
6	32.195908	-70.811484	.76679126+02	20	56.749992	-86.865145	.76777051+02
81	155.001493	59.500465	.76682099+02	85	157.317680	-59.138287	.76793378+02
82	155.002668	-120.497656	.76682099+02	86	157.317898	120.858227	.76793378+02
31	76.765212	-48.685367	.76684966+02	87	179.999275	22.224597	.76806664+02
32	76.765677	131.314968	.76684966+02	59	114.771196	-47.640540	.76841180+02
79	139.582048	92.048113	.76686942+02	60	114.771701	132.358852	.76841179+02
80	139.582573	-87.950284	.76686943+02	83	157.238739	1.993498	.76866220+02
45	95.633071	-34.803135	.76691522+02	84	157.240093	-178.007765	.76866219+02
46	95.633853	145.196758	.76691522+02	39	79.609020	21.936519	.76870116+02
9	35.842771	-31.142356	.76700783+02	40	79.610466	-158.063477	.76870116+02
10	35.843616	148.859249	.76700784+02	11	39.712418	73.715937	.76871612+02
15	54.219216	-60.505955	.76701559+02	12	39.713317	-106.285409	.76871612+02
16	54.219386	119.495087	.76701559+02	53	98.391078	74.627445	.76878450+02
37	77.811253	83.352783	.76701941+02	54	98.391980	-105.372405	.76878449+02
38	77.811966	-96.647509	.76701940+02	23	58.154878	-34.820674	.76883157+02
43	94.659920	37.891381	.76703771+02	24	58.155649	145.180090	.76883157+02
44	94.661319	-142.108589	.76703770+02				

Total Coulomb Energy: 3337.00075001

## 88 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
17	54.667302	-48.655501	.77533927+02	71	125.853777	-167.689556	.77648536+02
18	54.667304	131.344498	.77533929+02	72	125.856514	12.311375	.77648579+02
81	147.315512	-156.693659	.77543077+02	73	129.686005	94.186872	.77650458+02
82	147.318104	23.308043	.77543096+02	74	129.686951	-85.812658	.77650460+02
1	13.189660	-71.086602	.77548102+02	50	96.678737	-44.390863	.77651509+02
2	13.189928	108.918375	.77548101+02	49	96.677678	135.606941	.77651532+02
68	119.333441	-110.621319	.77552726+02	65	117.891930	117.436172	.77657399+02
67	119.333108	69.377798	.77552736+02	66	117.892941	-62.562339	.77657430+02
45	95.503992	73.241281	.77552944+02	37	80.101425	55.793441	.77658094+02
46	95.504655	-106.756403	.77552941+02	38	80.101645	-124.203635	.77658117+02
69	125.501171	-138.881916	.77553265+02	64	117.565552	-36.547187	.77660803+02
70	125.502573	41.119002	.77553297+02	63	117.563824	143.451292	.77660861+02
36	77.566843	170.705917	.77565613+02	13	42.734506	32.985708	.77662182+02
35	77.566428	-9.294742	.77565645+02	14	42.735243	-147.013968	.77662185+02
32	75.536518	-33.792674	.77569496+02	23	60.498736	7.623801	.77664391+02
31	75.536057	146.206825	.77569509+02	24	60.499974	-172.375509	.77664384+02
19	56.416930	-20.853873	.77582600+02	8	33.070369	144.994955	.77664413+02
20	56.417575	159.146694	.77582599+02	7	33.069635	-35.006453	.77664436+02
55	104.464747	51.201843	.77583315+02	78	138.862570	-14.800789	.77666724+02
56	104.464774	-128.796467	.77583317+02	77	138.860786	165.199659	.77666748+02
79	142.031069	-117.738247	.77589068+02	27	65.832699	32.635313	.77670282+02
80	142.031906	62.264072	.77589077+02	28	65.832910	-147.363829	.77670304+02
25	62.226475	104.725162	.77606384+02	75	137.846130	130.761347	.77683026+02
26	62.226721	-75.274001	.77606374+02	76	137.847912	-49.239711	.77683021+02
59	107.304327	92.322958	.77616531+02	86	160.170988	-26.749309	.77687504+02
60	107.305301	-87.674989	.77616534+02	85	160.168737	153.252157	.77687526+02
3	18.365847	16.824181	.77617750+02	22	57.017496	-123.866121	.77695251+02
4	18.367062	-163.176346	.77617744+02	21	57.016739	56.133015	.77695269+02
5	30.969260	65.506742	.77619493+02	29	72.407271	77.509219	.77711141+02
6	30.969849	-114.494016	.77619501+02	30	72.407734	-102.488106	.77711140+02
48	96.057789	-21.758632	.77625786+02	40	82.248358	-165.952749	.77718393+02
47	96.056690	158.239788	.77625803+02	39	82.247414	14.045598	.77718433+02
57	107.035486	-155.159517	.77631861+02	51	96.686091	113.305681	.77794300+02
58	107.037316	24.839879	.77631874+02	52	96.687077	-66.691810	.77794323+02
41	83.643172	96.053329	.77636860+02	62	116.934296	-12.069195	.77800128+02
42	83.644272	-83.944286	.77636867+02	61	116.932962	167.928986	.77800160+02
9	37.586432	107.979445	.77640149+02	83	151.078773	100.054523	.77814948+02
10	37.586476	-72.021255	.77640174+02	84	151.080086	-79.949242	.77814958+02
53	100.160069	-177.708670	.77642077+02	44	88.170940	35.513532	.77815574+02
54	100.160528	2.292128	.77642090+02	43	88.170267	-144.483643	.77815591+02
87	167.721594	-124.543296	.77644061+02	15	50.624862	82.150889	.77825522+02
88	167.722990	55.468471	.77644059+02	16	50.625139	-97.848879	.77825540+02
34	76.381246	-57.277554	.77645202+02	12	39.507537	-179.999271	.77831703+02
33	76.380760	122.721326	.77645225+02	11	39.506230	.000000	.77831719+02

Total Coulomb Energy: 3416.73289042

89 POINTS  
C<sub>2</sub> (LOWEST MIN)

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
34	81.606621	-178.779236	.78464277+02	50	100.945364	-166.624100	.78591472+02
35	81.606623	1.220761	.78464284+02	51	100.945387	13.375843	.78591475+02
28	66.116072	-39.579046	.78465830+02	84	148.731644	-119.724756	.78594037+02
29	66.116135	140.420952	.78465826+02	85	148.731695	60.275061	.78594037+02
82	147.402933	-18.342908	.78484948+02	24	63.217111	-13.653193	.78595637+02
83	147.403044	161.657225	.78484945+02	25	63.217130	166.346766	.78595630+02
88	167.586552	23.218541	.78496617+02	74	127.485250	-131.512415	.78595999+02
89	167.586569	-156.780853	.78496616+02	75	127.485271	48.487535	.78595998+02
26	63.290194	-138.462433	.78500147+02	76	136.297110	-51.452073	.78596914+02
27	63.290306	41.537602	.78500148+02	77	136.297256	128.547960	.78596914+02
48	96.411228	-68.978884	.78509524+02	10	41.742499	-147.950527	.78597315+02
49	96.411365	111.021208	.78509525+02	11	41.742603	32.049562	.78597316+02
32	72.740841	-64.886065	.78515712+02	30	67.719845	-111.898394	.78598311+02
33	72.740959	115.113997	.78515710+02	31	67.719949	68.101635	.78598311+02
44	87.468894	-47.645159	.78518524+02	60	107.061169	-119.502981	.78600121+02
45	87.469002	132.354614	.78518521+02	61	107.061209	60.497040	.78600120+02
38	82.521646	-153.592838	.78519851+02	62	112.333432	-51.937741	.78602537+02
39	82.521721	26.407184	.78519852+02	63	112.333556	128.062338	.78602536+02
22	63.142352	-164.709074	.78529283+02	58	104.665663	-92.238541	.78608647+02
23	63.142415	15.290975	.78529287+02	59	104.665780	87.761513	.78608646+02
56	103.332024	-8.749153	.78536944+02	36	82.015959	-86.465376	.78620545+02
57	103.332084	171.250917	.78536937+02	37	82.016103	93.534732	.78620545+02
12	43.328958	-32.011375	.78537330+02	70	124.680826	-103.830832	.78627758+02
13	43.329005	147.988495	.78537325+02	71	124.680900	76.169144	.78627757+02
86	161.071106	-63.479105	.78537537+02	64	119.708813	-74.876242	.78638991+02
87	161.071238	116.520825	.78537537+02	65	119.708947	105.123801	.78638990+02
1	.000000	84.999987	.78545662+02	4	23.088636	-179.032274	.78648515+02
80	143.703051	20.434861	.78556866+02	5	23.088672	.968087	.78648515+02
81	143.703056	-159.564968	.78556863+02	16	46.837127	-116.976504	.78650807+02
7	24.218077	124.927073	.78564449+02	17	46.837246	63.023512	.78650805+02
6	24.217965	-55.072653	.78564461+02	68	124.305821	-27.310361	.78654629+02
20	60.550676	-87.977367	.78566036+02	69	124.305936	152.689703	.78654626+02
21	60.550840	92.022647	.78566033+02	66	120.915507	-156.477024	.78740844+02
42	84.118194	-130.102358	.78570740+02	67	120.915533	23.522908	.78740846+02
43	84.118290	49.897692	.78570739+02	46	88.677630	-107.726616	.78741120+02
18	50.978226	-60.311188	.78574267+02	47	88.677705	72.273475	.78741118+02
19	50.978335	119.688750	.78574263+02	8	38.813121	-86.544489	.78749053+02
3	22.877230	60.803172	.78576929+02	9	38.813290	93.455459	.78749047+02
2	22.877094	-119.196953	.78576943+02	52	102.754847	-31.337515	.78771699+02
72	125.146664	-1.485494	.78583015+02	53	102.754952	148.662571	.78771695+02
73	125.146721	178.514593	.78583010+02	78	141.147900	-83.886658	.78775191+02
40	83.032306	-22.646335	.78583625+02	79	141.148014	96.113275	.78775191+02
41	83.032368	157.353685	.78583618+02	14	44.782669	179.999872	.78783826+02
54	103.094827	-142.176027	.78589781+02	15	44.782701	.000000	.78783831+02
55	103.094887	37.823958	.78589781+02				

Total Coulomb Energy: 3497.43901863

89 POINTS  
C<sub>2</sub> (NOT LOWEST MIN)

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
7	33.443293	-69.492292	.78458365+02	26	61.238385	-163.597143	.78586832+02
8	33.450958	110.546535	.78458367+02	35	78.455437	-49.890498	.78590069+02
71	123.191902	1.966401	.78473213+02	36	78.471429	130.114269	.78590065+02
72	123.218715	-178.033995	.78473222+02	51	97.432354	-36.306682	.78595745+02
31	75.313418	-73.677626	.78473841+02	52	97.453178	143.691368	.78595744+02
32	75.319298	106.329650	.78473836+02	59	110.423686	55.430327	.78604174+02
21	60.637336	65.022774	.78476594+02	60	110.440706	-124.562218	.78604173+02
22	60.650299	-114.990618	.78476595+02	67	118.799741	-25.409676	.78604609+02
73	132.905634	55.770374	.78481363+02	68	118.823560	154.583408	.78604609+02
74	132.922598	-124.210141	.78481360+02	75	136.077967	-53.330451	.78605511+02
55	101.766511	-10.755053	.78500435+02	76	136.092863	126.646362	.78605502+02
56	101.792517	169.243565	.78500433+02	69	119.238712	79.557227	.78609441+02
63	117.805657	31.160915	.78503191+02	70	119.245530	-100.428502	.78609440+02
64	117.829928	-148.832838	.78503188+02	39	81.675316	-.004863	.78610116+02
17	55.089930	92.466991	.78503424+02	40	81.702076	179.995335	.78610114+02
18	55.090635	-87.551910	.78503423+02	15	49.061127	40.200974	.78611108+02
33	76.307027	82.750459	.78508151+02	16	49.082625	-139.812843	.78611108+02
34	76.312304	-97.256402	.78508150+02	13	41.067189	3.071627	.78627248+02
19	55.534094	-60.337672	.78511545+02	14	41.093861	-176.927952	.78627247+02
20	55.545806	119.679005	.78511548+02	23	60.715284	-9.859053	.78633210+02
57	103.316084	12.924383	.78519717+02	24	60.741284	170.144548	.78633212+02
58	103.342478	-167.074570	.78519720+02	47	96.388535	-62.032043	.78644385+02
9	37.947519	72.402911	.78528874+02	48	96.399678	117.965668	.78644381+02
10	37.957331	-107.629025	.78528874+02	85	157.442904	-59.468225	.78644541+02
65	118.132872	-75.070415	.78543429+02	86	157.455147	120.472798	.78644546+02
66	118.138194	104.915802	.78543427+02	3	19.810410	-20.062144	.78648516+02
79	139.310211	91.472530	.78553221+02	4	19.834744	159.967861	.78648517+02
80	139.311367	-88.496116	.78553225+02	37	81.301520	-22.713251	.78650570+02
77	138.771582	23.442676	.78556229+02	38	81.325465	157.288542	.78650568+02
78	138.797461	-156.547335	.78556222+02	29	70.939660	41.002137	.78657918+02
83	155.017920	60.520122	.78571643+02	30	70.961000	-139.003536	.78657920+02
84	155.033045	-119.430848	.78571645+02	89	179.986141	4.081827	.78688563+02
49	96.749858	-83.885983	.78578854+02	53	97.816838	74.621279	.78750847+02
50	96.750973	96.111322	.78578850+02	54	97.825905	-105.375706	.78750845+02
81	139.912640	-19.509452	.78580307+02	41	83.030341	21.677397	.78761672+02
82	139.937716	160.478380	.78580300+02	42	83.055727	-158.323645	.78761676+02
43	83.678585	58.798921	.78583687+02	27	62.267235	-35.061792	.78761903+02
44	83.694172	-121.203870	.78583685+02	28	62.287954	144.947121	.78761909+02
11	40.876071	-32.960989	.78584342+02	87	157.778772	3.343287	.78762514+02
12	40.897398	147.057568	.78584347+02	88	157.806494	-176.657480	.78762520+02
46	95.987754	-141.122341	.78586718+02	61	115.080209	-50.046253	.78766004+02
45	95.965558	38.876326	.78586729+02	62	115.096354	129.943874	.78766004+02
1	12.320596	81.183050	.78586740+02	5	27.953152	34.675574	.78788122+02
2	12.326463	-98.935867	.78586740+02	6	27.976037	-145.350117	.78788122+02
25	61.212318	16.406102	.78586825+02				

Total Coulomb Energy: 3497.52321530

## 90 POINTS

 $D_2$ 

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
18	57.432797	40.071194	.79421012+02	81	139.706041	150.756514	.79524296+02
72	122.521467	-50.170087	.79421086+02	80	139.610317	-29.199002	.79524403+02
73	122.572988	129.815109	.79421654+02	10	40.328712	19.107402	.79524538+02
19	57.472281	-139.967451	.79421717+02	45	83.767127	-104.233414	.79528898+02
74	133.693680	76.829331	.79434430+02	47	96.239264	94.105534	.79528971+02
16	46.288745	-87.012717	.79434503+02	44	83.762199	75.815454	.79529742+02
17	46.314341	93.053524	.79434603+02	46	96.231137	-85.936275	.79529740+02
75	133.700438	-103.117018	.79434662+02	84	155.572107	71.877103	.79530650+02
35	78.484913	-152.197912	.79449964+02	6	24.406283	-82.127135	.79530661+02
57	101.569549	142.069508	.79449981+02	85	155.594547	-107.899228	.79530778+02
34	78.419374	27.848574	.79450459+02	7	24.426414	97.917460	.79530814+02
56	101.526137	-37.972814	.79450601+02	24	61.148731	12.930640	.79545799+02
58	102.108885	-61.095075	.79456883+02	66	118.786656	-23.049934	.79545897+02
32	77.853309	50.975517	.79456933+02	25	61.180732	-167.063528	.79546812+02
33	77.889901	-129.078131	.79457087+02	67	118.879568	156.930977	.79546822+02
59	102.147002	118.945085	.79457087+02	43	82.100329	-177.437204	.79553709+02
26	61.838498	67.855074	.79472158+02	49	97.963614	167.316719	.79553745+02
64	118.147766	-77.946703	.79472219+02	48	97.859501	-12.717588	.79554159+02
65	118.165611	102.055426	.79472369+02	42	82.075957	2.593624	.79554387+02
27	61.849523	-112.214972	.79472498+02	60	111.614004	78.134479	.79567426+02
83	139.902626	-139.008610	.79495428+02	31	68.398214	91.785218	.79567565+02
9	40.144684	128.941938	.79495529+02	30	68.369282	-88.286669	.79567636+02
8	40.113472	-51.084283	.79495682+02	61	111.614932	-101.884050	.79567780+02
82	139.839468	40.912330	.79495779+02	5	22.799799	-21.574998	.79579056+02
70	119.845172	26.992521	.79496863+02	86	157.139713	11.428509	.79579228+02
20	60.102001	-37.138836	.79496939+02	4	22.796921	158.391745	.79579949+02
21	60.145442	142.891609	.79497057+02	87	157.265549	-168.477161	.79579961+02
71	119.910254	-152.993244	.79497085+02	53	98.432815	-163.843124	.79603968+02
13	40.869450	-119.493153	.79501891+02	39	81.628295	153.727076	.79604023+02
79	139.152597	109.300249	.79501909+02	52	98.364823	16.221809	.79606500+02
78	139.117765	-70.627327	.79502350+02	38	81.579687	-26.357235	.79606523+02
12	40.861742	60.574797	.79502403+02	1	.000000	-153.434948	.79635832+02
15	43.918439	-14.441115	.79508495+02	90	179.936663	.000000	.79635846+02
76	136.022539	4.307059	.79508545+02	62	114.814238	1.577972	.79660955+02
22	60.223104	-63.484852	.79509503+02	29	65.128297	-11.712057	.79661016+02
68	119.739949	53.328140	.79509525+02	28	65.109972	168.301197	.79662434+02
14	43.909327	165.551115	.79509654+02	63	114.954532	-178.418697	.79662466+02
77	136.154613	-175.661839	.79509704+02	51	98.241448	-119.740376	.79679423+02
23	60.261124	116.570804	.79510186+02	41	81.784827	109.630873	.79679567+02
69	119.772933	-126.662730	.79510204+02	40	81.749704	-70.445117	.79679920+02
55	99.264668	-141.555939	.79516570+02	50	98.220679	60.302721	.79680090+02
37	80.782436	131.443962	.79516680+02	3	22.030507	-140.117350	.79725522+02
36	80.737563	-48.633930	.79517428+02	89	158.010492	129.877905	.79725512+02
54	99.214874	38.493725	.79517490+02	88	157.935207	-49.935818	.79725638+02
11	40.350940	-160.909710	.79524257+02	2	22.022557	39.945155	.79725763+02

(note: not fully relaxed)

Total Coulomb Energy: 3579.17674107



## 91 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
59	107.291909	143.513004	.80351566+02	7	32.298476	90.183095	.80471944+02
60	107.301762	-36.478900	.80351562+02	62	110.159122	-79.415535	.80474063+02
79	137.310696	- .886520	.80361597+02	61	110.135328	100.580988	.80474116+02
80	137.318861	179.083954	.80361617+02	50	93.848037	-99.763894	.80477206+02
1	12.118514	51.750554	.80364007+02	49	93.819360	80.236926	.80477225+02
2	12.144790	-128.185017	.80364002+02	65	115.865421	-13.576937	.80479511+02
17	52.842172	73.615208	.80366467+02	66	115.867274	166.408438	.80479535+02
18	52.870828	-106.386409	.80366496+02	14	43.781418	-23.201481	.80479978+02
91	179.986685	70.673096	.80376164+02	13	43.776838	156.829029	.80479993+02
39	83.120422	42.059284	.80393569+02	82	140.202341	-115.320456	.80482048+02
40	83.144752	-137.941151	.80393582+02	81	140.175604	64.684686	.80482064+02
41	83.195393	138.768526	.80403091+02	10	35.452157	-128.233892	.80482655+02
42	83.208936	-41.233335	.80403114+02	9	35.426281	51.750168	.80482667+02
27	68.400410	158.092197	.80405642+02	74	131.012592	-31.550308	.80487051+02
28	68.404803	-21.917057	.80405670+02	73	131.006268	148.425898	.80487074+02
85	155.599741	30.458064	.80415584+02	30	69.886404	-156.968866	.80490028+02
86	155.620277	-149.581251	.80415576+02	29	69.868927	23.024759	.80490045+02
35	76.191338	65.081061	.80416277+02	31	71.533656	87.871953	.80493209+02
36	76.219915	-114.920231	.80416321+02	32	71.561757	-92.133213	.80493292+02
45	91.288110	159.352810	.80417295+02	37	77.375894	- .035329	.80494436+02
46	91.291344	-20.644845	.80417299+02	38	77.383555	179.968517	.80494429+02
25	60.754047	48.326376	.80422315+02	89	158.196808	90.454267	.80496488+02
26	60.779762	-131.668503	.80422326+02	90	158.221878	-89.523805	.80496479+02
87	156.321489	155.911478	.80424555+02	23	60.505970	135.338825	.80503306+02
88	156.323954	-24.026677	.80424558+02	24	60.521673	-44.673053	.80503380+02
68	116.849223	-166.536968	.80427069+02	75	131.996466	94.425864	.80509845+02
67	116.835262	13.476826	.80427084+02	76	132.021818	-85.564678	.80509840+02
69	119.948757	122.683447	.80432651+02	64	115.490859	-103.345398	.80512974+02
70	119.966046	-57.305186	.80432642+02	63	115.462242	76.655239	.80512985+02
51	97.447541	122.241620	.80433073+02	21	55.617064	.177179	.80545048+02
52	97.465596	-57.756537	.80433065+02	22	55.624904	-179.804430	.80545070+02
19	54.797268	103.094408	.80436865+02	47	91.472855	20.242051	.80545907+02
20	54.824220	-76.917081	.80436884+02	48	91.489263	-159.761051	.80545899+02
4	19.201681	-41.196589	.80444560+02	44	88.613206	-78.281708	.80612132+02
3	19.186019	138.877701	.80444627+02	43	88.589927	101.719377	.80612179+02
33	73.352930	116.666014	.80446046+02	71	120.261083	52.997625	.80637294+02
34	73.373546	-63.338800	.80446041+02	72	120.286910	-127.010195	.80637308+02
53	98.216418	58.088182	.80453759+02	12	40.345347	-55.153238	.80638103+02
54	98.243704	-121.914342	.80453770+02	11	40.323661	124.874184	.80638156+02
6	29.960568	-173.101583	.80456670+02	83	142.327620	121.800976	.80656637+02
5	29.951045	6.851878	.80456690+02	84	142.344875	-58.171303	.80656656+02
57	106.656787	35.188424	.80468411+02	55	99.024105	- .033006	.80669528+02
58	106.678371	-144.818928	.80468416+02	56	99.032028	179.960455	.80669520+02
77	133.290901	30.923352	.80470186+02	16	48.391423	-153.896715	.80674608+02
78	133.311600	-149.095509	.80470187+02	15	48.373286	26.085109	.80674631+02
8	32.327378	-89.827584	.80471913+02				

Total Coulomb Energy: 3661.71369933

## 92 POINTS

 $C_2$ 

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
17	52.840603	157.622330	.81302591+02	67	116.286662	-24.959474	.81419226+02
18	52.840737	-22.369202	.81302592+02	68	116.287045	155.045940	.81419225+02
1	12.042437	-179.030951	.81303222+02	13	43.770598	-103.360515	.81427165+02
2	12.046952	1.015907	.81303222+02	14	43.781464	76.637527	.81427166+02
71	122.455555	-69.521304	.81311133+02	37	75.970887	-126.804831	.81427454+02
72	122.463696	110.483483	.81311132+02	38	75.981608	53.195951	.81427457+02
27	67.673291	-104.550628	.81315504+02	75	129.316202	-159.116861	.81427956+02
28	67.684225	75.448788	.81315503+02	76	129.323828	20.876642	.81427955+02
89	158.893608	-29.285385	.81318619+02	61	111.776471	-48.148587	.81429549+02
90	158.894989	150.743340	.81318616+02	62	111.781242	131.855343	.81429550+02
59	106.634404	-89.942986	.81331452+02	9	35.010943	179.984930	.81429812+02
60	106.644703	90.058267	.81331450+02	10	35.015274	-0.000551	.81429811+02
41	83.211066	-84.933632	.81331584+02	51	96.657599	173.703659	.81430611+02
42	83.220834	95.065806	.81331583+02	52	96.660751	-6.297432	.81430612+02
39	81.188711	-169.942566	.81333585+02	65	113.749640	-112.864311	.81432471+02
40	81.194770	10.059026	.81333585+02	66	113.760805	67.135676	.81432471+02
79	134.209110	-42.524201	.81347048+02	7	32.443339	-38.059408	.81434470+02
80	134.212851	137.485996	.81347049+02	8	32.446148	141.923830	.81434472+02
35	75.316830	166.568806	.81350110+02	73	129.185095	-94.940615	.81440185+02
36	75.318677	-13.428208	.81350112+02	74	129.195786	85.062120	.81440181+02
45	90.024372	-105.734687	.81355272+02	77	131.121572	-129.232218	.81440238+02
46	90.035378	74.265429	.81355273+02	78	131.132404	50.765115	.81440236+02
55	99.082780	-69.106229	.81357134+02	57	103.772927	-163.909304	.81444179+02
56	99.090840	110.894922	.81357135+02	58	103.779939	16.088773	.81444177+02
23	59.538799	-176.570148	.81363069+02	29	68.380769	-150.482979	.81447971+02
24	59.543748	3.435776	.81363070+02	30	68.389556	29.519804	.81447971+02
87	150.915575	-156.577951	.81369707+02	91	169.529455	-111.329117	.81459187+02
88	150.923580	23.408118	.81369708+02	92	169.540770	68.671720	.81459189+02
21	55.278633	-51.013039	.81374875+02	43	89.320852	-147.410313	.81485211+02
22	55.283761	128.980133	.81374877+02	44	89.330008	32.589906	.81485210+02
83	146.301991	-70.299389	.81377084+02	63	112.441486	-142.239214	.81486528+02
84	146.310244	109.712026	.81377085+02	64	112.451203	37.758763	.81486524+02
81	138.792997	168.928415	.81378826+02	19	54.667876	-127.322502	.81491617+02
82	138.795181	-11.083953	.81378828+02	20	54.678576	52.679472	.81491619+02
33	74.573107	-63.323596	.81378941+02	47	90.201013	-48.945254	.81559790+02
34	74.580259	116.674070	.81378944+02	48	90.205917	131.054672	.81559792+02
3	19.154465	-85.379953	.81394495+02	69	118.182676	178.679976	.81578640+02
4	19.164146	94.605250	.81394496+02	70	118.186688	-1.325470	.81578643+02
5	29.537399	-133.449989	.81399515+02	85	148.482944	-111.002874	.81587876+02
6	29.547717	46.556764	.81399514+02	86	148.494282	68.997822	.81587875+02
31	72.271824	-36.145579	.81403546+02	11	40.389861	-72.080358	.81601291+02
32	72.274339	143.850849	.81403544+02	12	40.398105	107.911082	.81601293+02
49	94.432547	-27.796052	.81405056+02	53	97.201893	-126.435522	.81604842+02
50	94.433467	152.204679	.81405058+02	54	97.212623	53.564292	.81604845+02
25	60.811578	-81.497594	.81417110+02	15	47.326112	-153.715139	.81632853+02
26	60.820950	98.499216	.81417109+02	16	47.334489	26.291540	.81632853+02

Total Coulomb Energy: 3745.33860835

## 93 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
32	71.145055	81.169577	.82218639+02	68	118.686174	87.562591	.82349702+02
33	71.145057	-98.830420	.82218650+02	69	118.686483	-92.437032	.82349704+02
12	41.441748	45.235334	.82253392+02	55	100.934237	-135.429506	.82350555+02
13	41.441893	-134.764536	.82253398+02	54	100.933762	44.570182	.82350566+02
62	109.950345	64.930572	.82261116+02	18	50.309986	129.350079	.82352109+02
63	109.950791	-115.069154	.82261115+02	19	50.310170	-50.650023	.82352151+02
64	112.197900	140.101862	.82261663+02	30	69.637080	8.919794	.82354006+02
65	112.198057	-39.897893	.82261670+02	31	69.637963	-171.079029	.82354016+02
34	73.158118	123.320051	.82265337+02	50	94.803082	82.898273	.82355040+02
35	73.158379	-56.680419	.82265367+02	51	94.803349	-97.101680	.82355052+02
86	147.521080	-7.941021	.82267143+02	60	108.186207	22.984889	.82358127+02
87	147.521374	172.058249	.82267142+02	61	108.187065	-157.014992	.82358130+02
72	123.308484	41.763903	.82268863+02	84	146.035433	35.125735	.82359363+02
73	123.309045	-138.235849	.82268860+02	85	146.035889	-144.874340	.82359358+02
92	169.144640	21.358704	.82301975+02	44	86.328379	63.774117	.82365876+02
93	169.145052	-158.642868	.82301975+02	45	86.328651	-116.225696	.82365878+02
7	23.828333	-166.416899	.82302572+02	90	157.853071	128.214834	.82377439+02
6	23.827897	13.584078	.82302683+02	91	157.853220	-51.783789	.82377441+02
22	59.547530	-77.267808	.82308083+02	56	102.003448	-19.827880	.82378466+02
23	59.547808	102.732306	.82308079+02	57	102.003723	160.171953	.82378459+02
5	23.518383	69.715965	.82312713+02	76	130.154232	13.650553	.82382714+02
4	23.518355	-110.285246	.82312768+02	77	130.154745	-166.349758	.82382711+02
80	136.314014	135.997627	.82315617+02	38	80.063498	-15.072007	.82383611+02
81	136.314074	-44.001888	.82315620+02	39	80.064131	164.928175	.82383602+02
74	126.326694	-18.805596	.82315850+02	70	119.473866	117.415059	.82385795+02
75	126.326853	161.194031	.82315843+02	71	119.474006	-62.584787	.82385792+02
1	.000000	139.840626	.82317791+02	28	66.079041	145.904442	.82414223+02
16	47.786024	-102.922051	.82320936+02	29	66.079427	-34.096235	.82414281+02
17	47.786335	77.077579	.82320943+02	42	86.283629	24.080435	.82420426+02
15	45.228456	-168.432999	.82325214+02	43	86.284650	-155.918924	.82420429+02
14	45.227958	11.566381	.82325232+02	49	91.496265	-176.922670	.82430939+02
11	39.363801	156.508678	.82331131+02	48	91.495835	3.077027	.82430957+02
10	39.362481	-23.492637	.82331178+02	3	21.458039	133.800400	.82453515+02
78	132.706930	66.660959	.82331330+02	2	21.456290	-46.200617	.82453743+02
79	132.707411	-113.338628	.82331329+02	20	58.302797	-11.312041	.82492385+02
52	95.619611	123.297040	.82334445+02	21	58.304016	168.689463	.82492387+02
53	95.619814	-56.702953	.82334465+02	88	153.901222	75.914489	.82513508+02
41	81.345804	102.193508	.82335486+02	89	153.901751	-104.085052	.82513507+02
40	81.345772	-77.806776	.82335500+02	9	37.485004	104.948074	.82514395+02
46	87.988763	143.004375	.82341490+02	8	37.484499	-75.051159	.82514408+02
47	87.989047	-36.995669	.82341522+02	67	112.419219	179.999857	.82555131+02
82	137.623873	101.844614	.82343691+02	66	112.418916	.000000	.82555144+02
83	137.624233	-78.154904	.82343694+02	58	102.913004	103.075612	.82556230+02
26	62.437840	58.328946	.82347294+02	59	102.913028	-76.924300	.82556237+02
27	62.437860	-121.670636	.82347287+02	36	78.968247	43.676462	.82569151+02
24	60.914604	31.105798	.82348387+02	37	78.968489	-136.323149	.82569143+02
25	60.914937	-148.893581	.82348400+02				

Total Coulomb Energy: 3829.84433843

94 POINTS  
C<sub>s</sub> (Non Min)

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
10	37.876728	0.000000	.83147594E+02	53	100.743953	139.407064	.83290698E+02
79	130.243317	-180.000000	.83178972E+02	54	100.743953	-139.407063	.83290698E+02
3	20.523990	90.000000	.83187130E+02	31	69.492585	41.079091	.83299063E+02
4	20.523990	-90.000000	.83187131E+02	32	69.492585	-41.079091	.83299063E+02
51	93.104624	159.513869	.83193992E+02	49	91.438477	119.630832	.83299729E+02
52	93.104624	-159.513868	.83193992E+02	50	91.438477	-119.630832	.83299729E+02
46	88.009232	0.000000	.83209020E+02	23	60.672172	91.383874	.83302176E+02
88	150.311694	0.000000	.83212018E+02	24	60.672172	-91.383874	.83302177E+02
86	144.688707	79.934344	.83217270E+02	57	101.419484	18.610009	.83304556E+02
87	144.688707	-79.934344	.83217270E+02	58	101.419484	-18.610009	.83304556E+02
73	122.977446	89.773127	.83218368E+02	1	8.480876	-180.000000	.83308147E+02
74	122.977446	-89.773127	.83218368E+02	45	85.137403	-180.000000	.83309277E+02
35	76.961582	19.087999	.83223998E+02	2	12.795299	0.000000	.83312231E+02
36	76.961582	-19.087999	.83223998E+02	25	63.993543	67.185018	.83317088E+02
19	53.304581	21.520531	.83228173E+02	26	63.993543	-67.185018	.83317088E+02
20	53.304581	-21.520531	.83228173E+02	29	66.485833	117.824280	.83318818E+02
75	125.792091	62.586381	.83240363E+02	30	66.485833	-117.824279	.83318818E+02
76	125.792091	-62.586381	.83240363E+02	59	104.695678	74.541250	.83326329E+02
84	140.867561	41.028476	.83243486E+02	60	104.695678	-74.541250	.83326329E+02
85	140.867561	-41.028476	.83243486E+02	89	153.629086	-180.000000	.83333209E+02
13	44.437198	110.070133	.83247592E+02	65	112.724498	114.390337	.83336046E+02
14	44.437198	-110.070133	.83247592E+02	66	112.724498	-114.390336	.83336046E+02
37	78.624890	137.765917	.83251597E+02	41	82.960266	79.929260	.83346275E+02
38	78.624890	-137.765917	.83251598E+02	42	82.960266	-79.929260	.83346275E+02
67	115.932154	159.412667	.83252459E+02	43	84.529768	58.444958	.83350225E+02
68	115.932154	-159.412667	.83252459E+02	44	84.529768	-58.444958	.83350225E+02
27	64.150022	0.000000	.83253412E+02	77	129.650711	14.338881	.83386062E+02
11	40.864856	77.423319	.83260871E+02	78	129.650711	-14.338881	.83386062E+02
12	40.864856	-77.423319	.83260871E+02	47	91.158697	36.638784	.83392583E+02
82	139.522947	150.402073	.83271496E+02	48	91.158697	-36.638784	.83392583E+02
83	139.522947	-150.402073	.83271496E+02	15	48.061209	163.027133	.83395683E+02
92	162.359661	47.848943	.83271617E+02	16	48.061209	-163.027132	.83395683E+02
93	162.359661	-47.848943	.83271617E+02	55	101.002670	96.149014	.83395897E+02
33	71.288910	157.955422	.83272802E+02	56	101.002670	-96.149014	.83395897E+02
34	71.288910	-157.955421	.83272802E+02	64	111.700899	0.000000	.83419818E+02
8	30.895931	136.436440	.83272865E+02	94	175.245772	-180.000000	.83466412E+02
9	30.895931	-136.436439	.83272865E+02	17	49.081599	48.780503	.83467076E+02
6	29.572863	37.813296	.83272889E+02	18	49.081599	-48.780503	.83467076E+02
7	29.572863	-37.813296	.83272889E+02	71	121.708999	135.737177	.83468141E+02
90	156.514025	120.650304	.83273702E+02	72	121.708999	-135.737177	.83468141E+02
91	156.514025	-120.650303	.83273702E+02	61	105.651404	52.862732	.83484680E+02
63	106.467769	-180.000000	.83273711E+02	62	105.651404	-52.862732	.83484680E+02
21	54.933333	137.958234	.83274684E+02	28	64.408923	-180.000000	.83500306E+02
22	54.933333	-137.958234	.83274684E+02	5	29.243072	-180.000000	.83509397E+02
80	135.589823	113.363367	.83283755E+02	39	80.241581	101.295251	.83510545E+02
81	135.589823	-113.363367	.83283755E+02	40	80.241581	-101.295251	.83510546E+02
69	117.646338	34.723353	.83285269E+02				
70	117.646338	-34.723353	.83285269E+02				

Total Coulomb Energy: 3915.45281247

## 94 POINTS

D<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
32	70.717021	97.124774	.83170423+02	66	116.026798	-164.319792	.83292045+02
33	70.717021	-82.875226	.83170423+02	67	116.026799	15.680208	.83292045+02
62	109.282979	-97.124774	.83170423+02	10	39.603215	175.154100	.83292089+02
63	109.282979	82.875227	.83170423+02	11	39.603215	-4.845899	.83292089+02
12	41.746486	-118.215817	.83207402+02	84	140.396786	-175.154100	.83292089+02
13	41.746486	61.784183	.83207402+02	85	140.396786	4.845899	.83292089+02
82	138.253515	118.215818	.83207402+02	16	47.847864	92.593314	.83294107+02
83	138.253515	-61.784183	.83207402+02	17	47.847864	-87.406686	.83294107+02
1	.000000	.000000	.83225072+02	78	132.152136	-92.593314	.83294107+02
94	180.000000	30.000000	.83225073+02	79	132.152136	87.406686	.83294107+02
30	70.040007	140.705135	.83230359+02	40	79.654432	-176.950499	.83301351+02
31	70.040007	-39.294865	.83230358+02	41	79.654432	3.049501	.83301350+02
64	109.959993	-140.705135	.83230359+02	54	100.345567	176.950500	.83301350+02
65	109.959994	39.294865	.83230359+02	55	100.345568	-3.049500	.83301350+02
42	85.357474	160.388241	.83237477+02	38	79.494376	118.617062	.83301513+02
43	85.357475	-19.611760	.83237477+02	39	79.494376	-61.382938	.83301513+02
52	94.642525	-160.388241	.83237478+02	56	100.505624	-118.617062	.83301513+02
53	94.642526	19.611760	.83237477+02	57	100.505624	61.382938	.83301513+02
44	86.161538	-99.908428	.83258331+02	18	48.213514	146.288570	.83310548+02
45	86.161539	80.091572	.83258331+02	19	48.213514	-33.711431	.83310547+02
50	93.838462	99.908428	.83258331+02	76	131.786486	-146.288570	.83310548+02
51	93.838462	-80.091572	.83258330+02	77	131.786486	33.711431	.83310548+02
34	72.178569	-153.622032	.83258509+02	14	45.488340	-150.527220	.83330446+02
35	72.178569	26.377968	.83258508+02	15	45.488340	29.472781	.83330446+02
60	107.821431	153.622032	.83258508+02	80	134.511660	150.527220	.83330446+02
61	107.821431	-26.377968	.83258508+02	81	134.511660	-29.472781	.83330446+02
4	23.132556	84.994601	.83268658+02	46	88.430488	-139.446417	.83346071+02
5	23.132556	-95.005399	.83268658+02	47	88.430488	40.553585	.83346071+02
90	156.867445	95.005400	.83268658+02	48	91.569512	139.446417	.83346071+02
91	156.867445	-84.994601	.83268658+02	49	91.569512	-40.553584	.83346071+02
6	23.949664	29.970769	.83271712+02	2	21.573023	151.192848	.83354389+02
7	23.949664	-150.029230	.83271712+02	3	21.573023	-28.807151	.83354389+02
88	156.050337	150.029232	.83271712+02	92	158.426977	-151.192848	.83354390+02
89	156.050337	-29.970768	.83271712+02	93	158.426977	28.807151	.83354390+02
26	62.769786	-105.934042	.83288945+02	22	58.648228	-171.797213	.83455228+02
27	62.769786	74.065958	.83288945+02	23	58.648228	8.202788	.83455228+02
68	117.230214	105.934043	.83288945+02	72	121.351772	171.797213	.83455228+02
69	117.230214	-74.065958	.83288945+02	73	121.351772	-8.202788	.83455228+02
20	58.293873	118.833927	.83290437+02	36	79.027050	-120.587536	.83492768+02
21	58.293873	-61.166073	.83290437+02	37	79.027050	59.412464	.83492769+02
74	121.706127	-118.833927	.83290437+02	58	100.972950	120.587536	.83492768+02
75	121.706127	61.166073	.83290437+02	59	100.972951	-59.412464	.83492768+02
24	61.533481	-133.038212	.83291452+02	8	36.618498	119.792531	.83497839+02
25	61.533481	46.961789	.83291452+02	9	36.618498	-60.207469	.83497839+02
70	118.466519	133.038212	.83291452+02	86	143.381502	-119.792531	.83497839+02
71	118.466519	-46.961789	.83291452+02	87	143.381502	60.207469	.83497839+02
28	63.973202	164.319792	.83292046+02				
29	63.973202	-15.680208	.83292045+02				

Total Coulomb Energy: 3915.30926962

94 POINTS  
C<sub>3</sub> (Non Min)

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
94	179.999995	.000008	.83159440E+02	7	34.235070	161.557232	.83286590E+02
34	74.542013	-18.744770	.83201214E+02	8	34.235070	-78.442769	.83286590E+02
36	74.542013	101.255230	.83201214E+02	9	34.235070	41.557232	.83286590E+02
35	74.542013	-138.744770	.83201215E+02	79	133.444687	-166.195931	.83290805E+02
82	139.439328	161.290234	.83205623E+02	80	133.444687	-46.195931	.83290805E+02
83	139.439328	-78.709767	.83205623E+02	81	133.444687	73.804069	.83290805E+02
84	139.439328	41.290233	.83205623E+02	40	79.705787	-58.831211	.83323873E+02
1	13.248094	-93.825718	.83209160E+02	41	79.705787	61.168789	.83323873E+02
2	13.248094	26.174283	.83209160E+02	42	79.705787	-178.831211	.83323873E+02
3	13.248094	146.174282	.83209160E+02	52	98.348812	-76.307916	.83326109E+02
10	37.312201	4.308530	.83216965E+02	53	98.348812	43.692084	.83326109E+02
11	37.312201	124.308530	.83216965E+02	54	98.348812	163.692084	.83326109E+02
12	37.312200	-115.691471	.83216965E+02	22	59.053310	51.705849	.83326616E+02
61	109.348396	-115.190776	.83226088E+02	23	59.053310	171.705849	.83326616E+02
62	109.348396	4.809224	.83226088E+02	24	59.053310	-68.294151	.83326616E+02
63	109.348396	124.809224	.83226088E+02	70	119.337037	173.993794	.83326674E+02
55	99.026854	-137.645997	.83248222E+02	71	119.337037	-66.006206	.83326674E+02
56	99.026854	-17.645997	.83248222E+02	72	119.337037	53.993794	.83326674E+02
57	99.026855	102.354003	.83248222E+02	49	95.657220	-98.139866	.83331543E+02
67	116.928009	149.253205	.83258815E+02	50	95.657221	141.860134	.83331543E+02
68	116.928009	29.253205	.83258815E+02	51	95.657220	21.860134	.83331543E+02
69	116.928009	-90.746796	.83258815E+02	25	61.059939	.328525	.83331843E+02
43	86.757238	-.189011	.83260525E+02	26	61.059939	120.328525	.83331843E+02
44	86.757238	119.810989	.83260525E+02	27	61.059939	-119.671475	.83331844E+02
45	86.757238	-120.189011	.83260525E+02	16	50.622649	-21.557716	.83341470E+02
19	53.826068	146.477429	.83262444E+02	18	50.622649	98.442284	.83341470E+02
20	53.826068	-93.522571	.83262444E+02	17	50.622649	-141.557716	.83341471E+02
21	53.826068	26.477429	.83262444E+02	73	121.122594	-135.025634	.83363006E+02
28	66.285584	78.945641	.83264901E+02	74	121.122594	-15.025634	.83363006E+02
29	66.285584	-41.054359	.83264901E+02	75	121.122594	104.974367	.83363006E+02
30	66.285584	-161.054359	.83264901E+02	37	77.258110	-81.076061	.83367114E+02
4	25.732865	-31.628502	.83265323E+02	38	77.258110	158.923939	.83367114E+02
5	25.732865	-151.628502	.83265323E+02	39	77.258110	38.923939	.83367114E+02
6	25.732865	88.371498	.83265323E+02	58	100.592471	-54.541054	.83457167E+02
76	132.198451	131.177728	.83269043E+02	59	100.592471	65.458946	.83457167E+02
78	132.198451	-108.822272	.83269043E+02	60	100.592471	-174.541054	.83457167E+02
77	132.198451	11.177728	.83269044E+02	13	44.880233	-168.971709	.83477843E+02
46	88.356245	-36.364867	.83270482E+02	14	44.880233	71.028291	.83477843E+02
47	88.356245	83.635133	.83270482E+02	15	44.880233	-48.971709	.83477843E+02
48	88.356245	-156.364867	.83270483E+02	85	142.075224	-17.413857	.83481735E+02
91	157.137227	70.365251	.83271670E+02	86	142.075224	102.586144	.83481735E+02
93	157.137227	-169.634748	.83271670E+02	87	142.075224	-137.413857	.83481735E+02
92	157.137227	-49.634749	.83271671E+02	31	74.423740	137.687195	.83490395E+02
88	157.051548	133.564312	.83277995E+02	32	74.423739	-102.312805	.83490395E+02
90	157.051547	-106.435688	.83277995E+02	33	74.423740	17.687195	.83490395E+02
89	157.051547	13.564312	.83277996E+02				
64	112.990432	-37.025053	.83283702E+02	Total Coulomb Energy: 3915.35216106			
65	112.990433	82.974947	.83283702E+02				
66	112.990433	-157.025052	.83283702E+02				

## 95 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
25	61.968044	20.749307	.84117815+02	2	10.778920	-45.366276	.84245246+02
26	61.968044	-159.250690	.84117813+02	17	50.437908	126.543047	.84247761+02
95	179.999998	.000218	.84143571+02	18	50.438003	-53.457023	.84247760+02
21	56.620288	-26.299206	.84143674+02	19	51.884395	95.969302	.84248271+02
22	56.620307	153.700815	.84143671+02	20	51.884569	-84.030724	.84248267+02
63	110.679145	117.530536	.84150707+02	27	63.981812	74.912487	.84248782+02
64	110.679254	-62.469558	.84150708+02	28	63.981902	-105.087613	.84248784+02
83	138.071278	-26.739219	.84155036+02	53	98.162311	52.983541	.84249417+02
84	138.071432	153.260550	.84155044+02	54	98.162427	-127.016572	.84249415+02
31	68.786452	176.778273	.84158046+02	39	78.249637	-24.744346	.84254429+02
32	68.786530	-3.221675	.84158045+02	40	78.249710	155.255577	.84254426+02
7	31.431320	105.707381	.84168530+02	45	89.024071	113.833828	.84255279+02
8	31.431479	-74.292700	.84168529+02	46	89.024190	-66.166356	.84255284+02
65	111.677184	73.329823	.84172761+02	93	158.505074	63.713326	.84255862+02
66	111.677259	-106.670342	.84172760+02	94	158.505161	-116.286394	.84255877+02
13	42.299904	68.190674	.84172831+02	9	34.551858	147.480377	.84257536+02
14	42.300006	-111.809286	.84172830+02	10	34.551903	-32.519776	.84257538+02
43	83.970104	-165.307713	.84181347+02	23	58.730862	47.901382	.84262178+02
44	83.970126	14.692299	.84181344+02	24	58.730939	-132.098656	.84262177+02
69	117.546544	-12.357690	.84184673+02	11	41.538236	32.657801	.84266295+02
70	117.546781	167.642361	.84184678+02	12	41.538256	-147.342100	.84266294+02
51	94.459958	134.496965	.84187434+02	77	132.428780	122.975931	.84266866+02
52	94.459961	-45.503230	.84187438+02	78	132.428831	-57.023954	.84266862+02
15	47.403712	179.422443	.84190159+02	3	21.531836	59.367410	.84271965+02
16	47.403771	-5.577609	.84190159+02	4	21.531915	-120.632336	.84271965+02
59	100.486623	95.253582	.84194842+02	81	134.108757	4.192727	.84273496+02
60	100.486723	-84.746576	.84194846+02	82	134.109058	-175.807350	.84273509+02
57	99.931806	30.793780	.84196130+02	79	133.409412	68.498519	.84276063+02
58	99.931915	-149.206343	.84196127+02	80	133.409473	-111.501515	.84276064+02
75	121.854403	95.730059	.84200880+02	47	90.378893	75.349360	.84282120+02
76	121.854481	-84.270020	.84200881+02	48	90.378951	-104.650723	.84282120+02
33	72.682110	134.281933	.84201977+02	71	118.601246	49.039740	.84302810+02
34	72.682172	-45.718032	.84201975+02	72	118.601364	-130.960472	.84302806+02
67	117.098196	-38.592818	.84212235+02	49	90.847337	174.153791	.84321294+02
68	117.098239	141.407202	.84212236+02	50	90.847468	-5.846207	.84321286+02
89	156.009552	4.554088	.84213396+02	55	99.894385	-24.929751	.84384532+02
90	156.009817	-175.445953	.84213426+02	56	99.894556	155.070450	.84384531+02
91	157.083683	-49.631279	.84215456+02	73	120.846128	24.798028	.84394807+02
92	157.083788	130.368313	.84215476+02	74	120.846225	-155.202250	.84394802+02
61	106.763863	-172.130501	.84221976+02	29	68.002668	112.194490	.84420416+02
62	106.763887	7.869648	.84221976+02	30	68.002806	-67.805469	.84420413+02
41	78.920782	36.210684	.84238419+02	37	77.831998	58.169961	.84446749+02
42	78.920873	-143.789366	.84238420+02	38	77.832108	-121.830126	.84446751+02
85	140.759109	37.643017	.84243864+02	5	26.047562	-173.669039	.84450119+02
86	140.759212	-142.356981	.84243871+02	6	26.047610	6.330736	.84450119+02
35	77.674059	92.572943	.84245160+02	87	143.517382	96.244442	.84450215+02
36	77.674096	-87.427122	.84245159+02	88	143.517422	-83.755475	.84450214+02
1	10.778792	134.634003	.84245247+02				

Total Coulomb Energy: 4001.77167557

## 96 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
44	85.027925	55.254765	.85098211+02	11	41.504035	73.374718	.85167942+02
43	85.027925	-124.745235	.85098224+02	12	41.520350	-106.569006	.85168006+02
7	31.967552	142.182388	.85108805+02	77	128.162889	-141.575834	.85171795+02
8	32.021991	-37.816888	.85108856+02	78	128.176876	38.464573	.85171807+02
93	160.241362	92.741622	.85113136+02	51	92.052978	115.237434	.85173153+02
94	160.271053	-87.363709	.85113159+02	52	92.094460	-64.767869	.85173163+02
22	53.445467	-43.617670	.85115464+02	31	69.925352	153.042641	.85182046+02
21	53.391380	136.378773	.85115525+02	32	69.975930	-26.957716	.85182174+02
83	136.957794	107.351262	.85118567+02	4	20.941111	-83.397864	.85191621+02
84	136.994850	-72.679162	.85118593+02	3	20.903831	96.493702	.85191650+02
27	62.764831	-116.996394	.85119487+02	2	10.681899	-6.243891	.85193697+02
26	62.758783	62.980083	.85119530+02	1	10.636117	173.895092	.85193775+02
76	126.804088	-45.969588	.85121570+02	95	169.321766	-178.095903	.85193874+02
75	126.759248	134.037243	.85121711+02	96	169.361666	2.056824	.85193923+02
58	101.300166	-109.354549	.85125584+02	81	130.305622	161.581579	.85195336+02
57	101.285445	70.658974	.85125627+02	82	130.353354	-18.405881	.85195371+02
14	41.791541	-72.038354	.85127335+02	66	110.205203	-25.459391	.85200468+02
13	41.745435	107.926042	.85127436+02	65	110.154963	154.537212	.85200478+02
49	90.418738	167.480612	.85128151+02	23	59.560181	87.887563	.85208686+02
50	90.466326	-12.514164	.85128257+02	24	59.588255	-92.088297	.85208706+02
41	80.515397	77.078156	.85128478+02	45	89.774090	-147.425062	.85211116+02
42	80.534849	-102.919884	.85128579+02	46	89.793411	32.577007	.85211129+02
64	109.626317	23.150448	.85130337+02	71	119.950041	87.477599	.85221385+02
63	109.598757	-156.866850	.85130363+02	72	119.977351	-92.547542	.85221394+02
89	148.982389	137.999563	.85136391+02	29	68.639698	-139.847933	.85238981+02
90	149.028902	-42.012236	.85136389+02	30	68.654482	40.135840	.85239081+02
68	110.960628	-2.212397	.85137384+02	80	128.897270	11.471760	.85253304+02
67	110.917465	177.775246	.85137506+02	79	128.861420	-168.559368	.85253391+02
33	70.566823	176.140648	.85139513+02	85	140.500816	74.682699	.85255141+02
34	70.610040	-3.866117	.85139509+02	86	140.518114	-105.371231	.85255204+02
70	114.597611	-69.125189	.85146042+02	9	32.857847	-176.456100	.85264455+02
69	114.558262	110.887656	.85146147+02	10	32.897346	3.489572	.85264561+02
55	99.141469	92.870728	.85146897+02	60	105.317491	-48.259127	.85275193+02
56	99.173654	-87.139566	.85147004+02	59	105.273872	131.745153	.85275439+02
17	50.487228	164.707855	.85150628+02	28	62.768799	-66.663474	.85282763+02
18	50.535861	-15.307487	.85150695+02	25	62.718566	113.322742	.85282994+02
54	92.250657	9.102997	.85159982+02	39	78.816002	99.033536	.85310516+02
53	92.214301	-170.902439	.85159995+02	40	78.852332	-80.966429	.85310765+02
20	52.687736	14.143833	.85160039+02	47	89.916391	146.058380	.85330076+02
19	52.656097	-165.826992	.85160088+02	48	89.967744	-33.935398	.85330312+02
61	105.790529	-133.212620	.85161182+02	36	73.105700	18.282266	.85333545+02
62	105.796601	46.803630	.85161227+02	35	73.077050	-161.707880	.85333637+02
91	149.352987	-138.839481	.85162021+02	74	121.507955	-117.483876	.85335895+02
92	149.365131	41.239398	.85162060+02	73	121.499267	62.548311	.85336006+02
15	47.699189	-138.691820	.85162858+02	6	26.891933	44.438875	.85339226+02
16	47.713518	41.263883	.85162880+02	5	26.880500	-135.455894	.85339315+02
37	76.532538	129.812059	.85166663+02	87	148.314632	179.957058	.85357350+02
38	76.585593	-50.181644	.85166658+02	88	148.356104	.000000	.85357435+02

Total Coulomb Energy: 4089.15401006



## 97 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
69	113.762187	-68.221052	.86011540+02	74	121.969982	-120.079474	.86123116+02
71	114.236232	111.852121	.86011669+02	34	70.709899	-23.927281	.86123541+02
47	86.720279	174.792475	.86041114+02	65	108.274885	173.447449	.86123972+02
46	86.686321	-5.184290	.86041609+02	64	108.220549	-6.710302	.86124683+02
40	80.266098	-45.284171	.86042186+02	70	113.858730	32.037324	.86135169+02
41	80.648990	134.667337	.86042357+02	68	113.603465	-147.783321	.86135724+02
76	124.292619	-169.367554	.86043769+02	43	81.324498	76.865766	.86136902+02
77	124.376800	10.305074	.86043778+02	42	80.828875	-103.124850	.86137325+02
1	.264927	99.506696	.86045345+02	39	79.081049	15.956363	.86139132+02
91	147.870432	143.093788	.86052521+02	60	102.786523	-47.794566	.86139332+02
90	147.556770	-37.534856	.86052549+02	62	103.172742	132.275019	.86139401+02
26	61.296648	-117.110533	.86055782+02	38	78.963132	-164.134514	.86139659+02
27	61.729975	62.980030	.86056305+02	54	99.438162	-85.610988	.86140662+02
84	136.050880	-72.454498	.86061504+02	55	99.942726	94.390192	.86140833+02
85	136.536135	107.687620	.86061536+02	22	57.842313	-42.834730	.86142811+02
72	120.116789	-92.792063	.86062929+02	23	58.230323	136.937153	.86143485+02
73	120.620461	87.180928	.86063088+02	48	90.219456	-146.244228	.86146343+02
15	45.916888	44.200803	.86065066+02	49	90.487133	33.746792	.86146675+02
14	45.588983	-136.131182	.86065230+02	51	91.065795	115.256325	.86150684+02
12	40.035250	-104.855254	.86065449+02	50	90.605578	-64.740329	.86151128+02
13	40.523839	75.307054	.86065614+02	24	59.802641	-92.489741	.86151506+02
6	23.304878	-135.260920	.86071849+02	25	60.326058	87.486952	.86152440+02
82	134.440382	-142.775702	.86072500+02	10	38.084737	-169.347933	.86165451+02
83	134.736866	36.824459	.86072740+02	11	38.114394	11.265452	.86165988+02
7	23.638123	45.661200	.86073278+02	81	130.701185	164.011471	.86167067+02
16	46.030265	-72.334108	.86082823+02	80	130.554291	-16.399083	.86167118+02
57	100.928621	13.713184	.86082952+02	3	21.341327	164.247040	.86184244+02
56	100.820308	-166.196791	.86083265+02	2	21.117842	-14.497588	.86185890+02
17	46.554891	107.490864	.86083669+02	95	158.294189	100.770170	.86190165+02
4	22.593304	-78.584102	.86085264+02	94	157.798197	-79.437546	.86190294+02
5	23.107905	101.272396	.86085640+02	87	140.003786	74.361814	.86195377+02
78	126.547224	-47.083607	.86090952+02	86	139.523991	-105.457294	.86195587+02
79	126.927000	133.162682	.86091037+02	45	82.979506	56.096104	.86200337+02
97	169.382515	172.050949	.86097001+02	44	82.595087	-123.906984	.86200723+02
96	169.292923	-10.586414	.86097162+02	28	64.938841	177.659685	.86210763+02
18	47.715655	-16.615029	.86098679+02	29	64.945030	-2.130358	.86212465+02
19	47.866351	162.917624	.86098973+02	8	36.819037	-43.886875	.86269869+02
31	67.099284	115.646448	.86099771+02	9	37.223247	135.568495	.86271055+02
30	66.619247	-64.258021	.86099900+02	21	57.519162	20.131070	.86272491+02
88	146.643299	-174.412836	.86102626+02	20	57.397642	-160.108513	.86274235+02
89	146.681311	4.822970	.86102748+02	92	154.901016	-133.174835	.86286120+02
58	102.068711	-107.111682	.86105834+02	93	155.261786	46.064449	.86286317+02
52	91.759277	-26.243563	.86105973+02	63	103.239443	51.141804	.86318293+02
53	91.994353	153.777985	.86106036+02	61	102.871882	-128.789246	.86318620+02
59	102.545771	72.850922	.86106300+02	37	78.928481	97.821634	.86327043+02
33	69.053307	39.465250	.86117292+02	36	78.423819	-82.146517	.86327817+02
32	68.767090	-140.633705	.86118468+02	66	112.484432	-28.537945	.86344950+02
35	70.926280	155.938330	.86122825+02	67	112.735403	151.639172	.86344948+02
75	122.392444	59.747968	.86122955+02				

Total Coulomb Energy: 4177.53360035

## 98 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
61	103.038757	-116.797955	.86963044+02	2	10.737312	.124088	.87064272+0
62	103.086886	63.203571	.86963044+02	73	122.242283	-70.033337	.87064893+0
21	56.083417	-160.278576	.86976354+02	74	122.270430	109.991677	.87064891+0
22	56.122921	19.740445	.86976354+02	89	145.587002	-167.039354	.87065793+0
63	108.787376	-51.569902	.86978388+02	90	145.622910	12.912783	.87065793+0
64	108.801501	128.445910	.86978387+02	85	137.859177	-94.060318	.87071859+0
13	41.739326	-64.475294	.86995860+02	86	137.901009	85.967011	.87071859+0
14	41.763498	115.477472	.86995860+02	41	79.987550	-78.247548	.87074991+0
81	130.003885	168.865295	.87002100+02	42	80.021062	101.746240	.87074991+0
82	130.023272	-11.172078	.87002101+02	25	58.822295	-114.517552	.87076045+0
7	31.095851	151.090244	.87006500+02	26	58.870129	65.477281	.87076045+0
8	31.100759	-28.829617	.87006500+02	45	87.833255	-58.348258	.87076588+0
97	167.997467	-167.456451	.87008705+02	46	87.852774	121.650056	.87076588+0
98	168.033113	12.387511	.87008705+02	65	109.321306	177.264513	.87086508+0
29	67.843113	-137.069618	.87014216+02	66	109.347013	-2.749901	.87086509+0
30	67.890574	42.934628	.87014217+02	11	40.066875	-100.301500	.87088302+0
19	51.819493	-37.991628	.87020750+02	12	40.111137	79.674700	.87088302+0
20	51.822319	141.970221	.87020750+02	95	162.014078	-77.409059	.87091266+0
57	101.616459	-75.194171	.87026886+02	96	162.047091	102.701169	.87091267+0
58	101.648046	104.813434	.87026885+02	69	111.692981	-137.863308	.87091657+0
17	50.112466	170.474108	.87029987+02	70	111.740320	42.132250	.87091657+0
18	50.133121	-9.489149	.87029988+02	15	46.016709	-136.110422	.87092301+0
39	78.310085	-156.344215	.87030414+02	16	46.064335	43.898887	.87092301+0
40	78.351441	23.661065	.87030416+02	91	149.565512	153.586128	.87097177+0
51	90.553949	-138.223640	.87035509+02	92	149.572439	-26.495768	.87097178+0
52	90.601209	41.776241	.87035509+02	33	69.931746	159.012272	.87098543+0
75	122.493391	-164.427382	.87037565+02	34	69.943254	-20.970468	.87098543+0
76	122.530774	15.552861	.87037565+02	77	124.648645	-116.348507	.87103011+0
59	102.060718	-157.617464	.87037857+02	78	124.696701	63.656370	.87103013+0
60	102.101490	22.376869	.87037859+02	3	21.019668	-74.970338	.87103516+0
9	34.544314	-168.287756	.87038506+02	4	21.051125	104.933381	.87103516+0
10	34.579504	11.760887	.87038506+02	31	69.671158	-178.561905	.87118503+0
79	127.892128	-40.193171	.87040792+02	32	69.699781	1.452642	.87118505+0
80	127.896822	139.844439	.87040790+02	23	57.602476	-85.442195	.87124855+0
71	115.635557	-94.043212	.87044202+02	24	57.640131	94.538311	.87124855+0
72	115.677378	85.968693	.87044202+02	53	92.926287	-36.435592	.87132913+0
55	94.942329	-96.792049	.87049969+02	54	92.927774	143.566881	.87132912+0
56	94.985298	83.209916	.87049969+02	47	89.932048	-174.555353	.87226003+0
43	81.924882	-119.070957	.87051896+02	48	89.963336	5.444678	.87226006+0
44	81.973239	60.928363	.87051896+02	35	73.034683	-42.296606	.87233196+0
67	111.111484	154.354246	.87053848+02	36	73.041131	137.688683	.87233196+0
68	111.119087	-25.664239	.87053850+02	83	132.390676	-141.246849	.87242055+0
49	90.155616	164.426901	.87057144+02	84	132.437305	38.740548	.87242056+0
50	90.171522	-15.573217	.87057146+02	37	74.495241	-99.269722	.87254510+0
93	150.316954	-123.750381	.87060688+02	38	74.539155	80.724503	.87254509+0
94	150.365606	56.251006	.87060689+02	5	25.511043	-129.087502	.87257724+0
27	63.900906	-62.254007	.87061697+02	6	25.559486	50.920329	.87257724+0
28	63.923415	117.724891	.87061697+02	87	142.137928	-62.228751	.87263102+0
1	10.709659	179.913126	.87064272+02	88	142.160440	117.826648	.87263101+0

Total Coulomb Energy: 4266.82246416

## 99 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
30	67.319370	-110.117626	.87894880+02	27	59.238576	122.032273	.88007105+02
31	67.319390	69.882386	.87894880+02	92	149.335514	-141.750126	.88007165+02
98	168.792400	-179.999542	.87918327+02	93	149.335577	38.249788	.88007168+02
99	168.792410	.000002	.87918328+02	64	105.617761	-168.308687	.88018119+02
62	104.941274	-50.490615	.87930386+02	65	105.617798	11.691338	.88018121+02
63	104.941319	129.509356	.87930384+02	10	38.611526	-6.103214	.88018969+02
12	39.926417	-72.454648	.87931476+02	11	38.611557	173.896717	.88018966+02
13	39.926447	107.545333	.87931475+02	86	139.338615	-74.274219	.88020480+02
58	99.484553	-9.974147	.87932770+02	87	139.338665	105.725807	.88020480+02
59	99.484556	170.025827	.87932768+02	14	44.420537	-39.412759	.88024058+02
46	84.681369	-172.283110	.87935359+02	15	44.420564	140.587191	.88024056+02
47	84.681398	7.716903	.87935362+02	94	151.116356	-43.485150	.88025318+02
96	161.096144	-92.923517	.87955979+02	95	151.116398	136.514927	.88025318+02
97	161.096239	87.076525	.87955981+02	54	95.969652	-71.934109	.88028295+02
34	69.555022	-152.562939	.87957370+02	55	95.969704	108.065864	.88028293+02
35	69.555044	27.437085	.87957372+02	24	59.174617	-85.915456	.88032388+02
52	90.958129	-31.582192	.87957870+02	25	59.174652	94.084532	.88032387+02
53	90.958157	148.417782	.87957869+02	42	80.798640	-92.232256	.88037784+02
38	78.211381	48.884746	.87959147+02	43	80.798690	87.767742	.88037784+02
39	78.211383	-131.115265	.87959145+02	44	83.877878	-52.112209	.88040614+02
80	127.405044	-131.050102	.87965738+02	45	83.877929	127.887761	.88040614+02
81	127.405119	48.949911	.87965739+02	18	48.160922	-158.802174	.88040627+02
48	89.597382	-111.773303	.87967753+02	19	48.160939	21.197846	.88040629+02
49	89.597404	68.226699	.87967754+02	78	126.584802	-50.142317	.88047849+02
66	111.815940	-28.585434	.87971599+02	79	126.584837	129.857683	.88047848+02
67	111.815966	151.414553	.87971597+02	28	63.970865	-175.314112	.88059808+02
82	129.999451	-160.316868	.87972774+02	29	63.970889	4.685926	.88059811+02
83	129.999475	19.683119	.87972776+02	72	116.362213	-71.755089	.88065805+02
1	.000000	157.195457	.87974351+02	73	116.362272	108.244871	.88065803+02
40	78.653536	-14.001440	.87974565+02	90	146.416006	179.151312	.88079602+02
41	78.653549	165.998533	.87974562+02	91	146.416006	-84.8766	.88079604+02
50	90.252212	-151.216375	.87978156+02	56	99.404008	48.945964	.88107758+02
51	90.252240	28.783628	.87978158+02	57	99.404017	-131.054028	.88107755+02
4	22.473946	-98.133658	.87980420+02	2	20.950460	16.644281	.88112294+02
5	22.473969	81.866379	.87980419+02	3	20.950495	-163.355791	.88112288+02
60	101.876767	-92.921442	.87981785+02	88	140.554802	-108.335225	.88121802+02
61	101.876830	87.078531	.87981784+02	89	140.554907	71.664784	.88121804+02
32	69.206766	-36.703496	.87986206+02	68	112.226430	-147.508619	.88137656+02
33	69.206804	143.296455	.87986205+02	69	112.226475	32.491421	.88137656+02
6	23.301352	-41.876156	.87989474+02	76	122.932638	-94.537596	.88159909+02
7	23.301378	138.123823	.87989469+02	77	122.932706	85.462339	.88159907+02
20	57.183475	-131.796057	.87991478+02	22	57.504753	-17.749474	.88165109+02
21	57.183476	48.203960	.87991480+02	23	57.504783	162.250458	.88165108+02
74	120.820113	176.061367	.88001338+02	8	36.070844	-133.747780	.88206505+02
75	120.820115	-3.938633	.88001342+02	9	36.070845	46.252218	.88206505+02
70	112.236632	-114.342859	.88004486+02	84	132.698757	-24.904796	.88211528+02
71	112.236659	65.657093	.88004486+02	85	132.698784	155.095228	.88211526+02
16	45.447691	-105.331230	.88007034+02	36	75.476723	-71.523280	.88229077+02
17	45.447705	74.668770	.88007033+02	37	75.476763	108.476703	.88229076+02
26	59.238542	-57.967692	.88007106+02				

Total Coulomb Energy: 4357.13916313

100 POINTS  
Almost Tetrahedral

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
100	179.999998	-72.395582	.88838394+02	29	64.204140	23.241685	.88941496+02
33	70.106204	-119.738061	.88838417+02	52	92.177333	-123.154132	.88941495+02
34	70.521028	.000002	.88838419+02	82	133.918623	-171.719980	.88942029+02
36	70.956665	120.258827	.88838439+02	51	91.634727	78.326846	.88942044+02
61	101.718830	-143.041761	.88911082+02	58	100.437612	-84.496879	.88942059+02
88	140.941214	-81.806547	.88911112+02	5	25.402606	13.996786	.88942070+02
12	36.354555	96.724303	.88911138+02	98	157.885923	-53.426940	.88947560+02
41	79.965152	39.299405	.88911129+02	18	49.007361	123.403878	.88947582+02
43	80.035969	159.449871	.88912821+02	42	80.035678	-140.226534	.88947575+02
89	141.080805	38.079384	.88912820+02	47	84.407303	17.683792	.88947593+02
10	35.731911	-143.699499	.88912838+02	25	59.471287	-70.634835	.88949908+02
62	101.932601	-23.330383	.88912839+02	72	116.017314	115.272476	.88949912+02
90	141.169561	158.888260	.88921504+02	86	134.680550	126.564266	.88949922+02
63	102.054279	96.664165	.88921520+02	19	50.666865	-47.589240	.88949960+02
11	35.783820	-22.718460	.88921535+02	85	134.527842	-114.048069	.88950005+02
40	79.826592	-80.700514	.88921549+02	21	51.538238	72.576633	.88950026+02
55	97.200646	176.692623	.88922164+02	27	59.489736	49.085015	.88950021+02
2	12.691286	-164.898211	.88922177+02	70	115.368415	-124.226277	.88950040+02
68	111.876464	-46.532848	.88922170+02	99	157.936745	-172.806042	.88950974+02
75	118.530928	50.047057	.88922184+02	17	48.670776	3.592949	.88951001+02
67	111.688912	-166.182718	.88927458+02	45	80.602075	99.752425	.88951024+02
3	13.117641	77.911956	.88927484+02	46	84.081760	-102.168530	.88951030+02
74	118.445499	-69.755283	.88927482+02	20	51.112955	-167.733829	.88954779+02
56	97.356357	56.283043	.88927521+02	26	59.486422	168.932652	.88954771+02
48	84.968910	137.886566	.88932866+02	71	115.601270	-4.564837	.88954780+02
96	157.824028	67.201208	.88932866+02	87	134.702442	5.793651	.88954811+02
44	80.159143	-20.681154	.88932877+02	79	122.740703	-146.304489	.89039124+02
16	48.131299	-116.225643	.88932891+02	76	121.560081	-93.540889	.89039150+02
22	57.423093	-140.029715	.88934030+02	9	32.848840	59.349930	.89039182+02
97	157.884192	9.344279	.88934022+02	38	77.049651	60.770095	.89039184+02
30	64.576850	143.175480	.88934036+02	37	76.874063	-179.094826	.89042992+02
53	92.366748	-3.508515	.88934040+02	8	32.616693	178.364632	.89043009+02
60	100.624125	155.519136	.88934061+02	81	122.958109	-26.689000	.89043006+02
4	25.206347	-106.992549	.88934085+02	77	121.692313	26.287206	.89043021+02
84	134.304136	67.805002	.88934081+02	80	122.882036	92.897079	.89058804+02
50	91.258024	-41.512249	.88934091+02	78	121.862419	147.286879	.89058823+02
23	57.686357	-20.241106	.88934144+02	7	31.817252	-60.529923	.89058884+02
54	92.909950	116.839648	.88934153+02	39	77.229191	-59.314960	.89058880+02
95	157.790556	129.323168	.88934147+02	31	69.858027	-39.622588	.89102544+02
28	63.766385	-96.560166	.88934185+02	66	105.588173	134.047537	.89102555+02
49	91.189581	-161.370445	.88938504+02	91	142.805334	97.937902	.89102564+02
6	25.829268	132.857132	.88938534+02	13	43.866587	-87.515906	.89102619+02
59	100.587155	35.240989	.88938551+02	15	44.454090	151.411272	.89123492+02
83	134.075876	-52.140997	.88938551+02	32	70.017443	-159.109135	.89123513+02
1	12.094888	-42.001951	.88940032+02	93	143.077019	-22.651374	.89123533+02
73	118.219398	170.843685	.88940026+02	65	104.837936	13.846066	.89123564+02
69	111.997980	73.018703	.88940046+02	14	44.190989	31.844729	.89124184+02
57	97.492048	-63.433618	.88940062+02	35	70.580655	80.855482	.89124194+02
94	157.675228	-110.721230	.88941463+02	92	142.877134	-142.458122	.89124194+02
24	58.136842	99.925407	.88941499+02	64	104.605635	-105.800629	.89124231+02

Total Coulomb Energy: 4448.35087922

100 POINTS  
TETRAHEDRAL

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
34	70.528772	.000000	.88838384+02	83	134.097916	67.805810	.88938158+02
35	70.528777	119.999997	.88838384+02	84	134.097918	-172.194181	.88938155+02
36	70.528777	-119.999997	.88838384+02	16	48.599966	3.410745	.88943987+02
100	179.999998	.000000	.88838379+02	17	48.599970	-116.589253	.88943987+02
10	35.955378	-23.410227	.88915133+02	18	48.599970	123.410743	.88943986+02
11	35.955380	96.589777	.88915132+02	43	80.271509	-20.558758	.88943985+02
12	35.955383	-143.410223	.88915131+02	44	80.271512	99.441240	.88943985+02
40	79.941479	39.178621	.88915131+02	45	80.271514	-140.558754	.88943984+02
41	79.941483	-80.821377	.88915131+02	46	84.485118	17.631449	.88943985+02
42	79.941484	159.178617	.88915127+02	47	84.485122	-102.368548	.88943985+02
61	101.905407	-23.409034	.88915129+02	48	84.485122	137.631447	.88943984+02
62	101.905410	96.590962	.88915130+02	97	157.879791	-53.193611	.88943982+02
63	101.905413	-143.409031	.88915128+02	98	157.879791	66.806373	.88943982+02
88	141.062469	38.210891	.88915129+02	99	157.879795	-173.193613	.88943980+02
89	141.062471	-81.789103	.88915128+02	19	51.112782	-47.753870	.88951605+02
90	141.062475	158.210888	.88915126+02	20	51.112784	72.746130	.88951604+02
1	12.632236	-43.186189	.88929282+02	21	51.112787	-167.753866	.88951601+02
2	12.632238	76.813829	.88929282+02	25	59.475623	48.949936	.88951604+02
3	12.632240	-163.186180	.88929281+02	26	59.475624	-71.050063	.88951604+02
55	97.347908	56.343002	.88929279+02	27	59.475627	168.949934	.88951600+02
56	97.347909	-63.656998	.88929280+02	70	115.660645	-4.671725	.88951602+02
57	97.347913	176.342999	.88929276+02	71	115.660648	-124.671721	.88951602+02
67	111.857453	-46.737164	.88929279+02	72	115.660648	115.328271	.88951602+02
68	111.857455	73.262835	.88929279+02	85	134.640327	5.922167	.88951602+02
69	111.857459	-166.737160	.88929276+02	86	134.640331	-114.077828	.88951601+02
73	118.398492	50.203959	.88929279+02	87	134.640331	125.922164	.88951601+02
74	118.398494	-69.796035	.88929279+02	7	32.432337	-61.113229	.89046751+02
75	118.398497	170.203959	.88929276+02	8	32.432337	58.886777	.89046751+02
22	57.752397	-20.287024	.88936726+02	9	32.432340	178.886770	.89046749+02
23	57.752399	99.712977	.88936726+02	37	77.044490	-59.387405	.89046749+02
24	57.752402	-140.287020	.88936725+02	38	77.044490	60.612593	.89046749+02
28	64.181005	23.107768	.88936726+02	39	77.044494	-179.387402	.89046745+02
29	64.181008	-96.892233	.88936725+02	76	121.708803	26.497999	.89046748+02
30	64.181010	143.107763	.88936724+02	77	121.708804	-93.501997	.89046748+02
52	92.483481	-3.445513	.88936724+02	78	121.708808	146.497993	.89046746+02
53	92.483485	-123.445510	.88936724+02	79	122.861983	-26.864156	.89046747+02
54	92.483485	116.554484	.88936724+02	80	122.861984	93.135840	.89046747+02
94	157.785818	9.138074	.88936721+02	81	122.861988	-146.864151	.89046747+02
95	157.785822	-110.861916	.88936721+02	13	44.166345	31.729597	.89117355+02
96	157.785822	129.138065	.88936721+02	14	44.166347	-88.270406	.89117355+02
4	25.475634	13.106518	.88938161+02	15	44.166350	151.729595	.89117353+02
5	25.475637	-106.893487	.88938161+02	31	70.157441	-39.461891	.89117354+02
6	25.475639	133.106518	.88938161+02	32	70.157443	80.538109	.89117353+02
49	91.363907	-41.692407	.88938159+02	33	70.157447	-159.461885	.89117351+02
50	91.363909	78.307591	.88938159+02	64	105.006783	13.861518	.89117352+02
51	91.363912	-161.692404	.88938156+02	65	105.006786	-106.138479	.89117352+02
58	100.549152	35.251141	.88938159+02	66	105.006787	133.861515	.89117351+02
59	100.549155	-84.748855	.88938159+02	91	142.922718	-22.570859	.89117351+02
60	100.549158	155.251139	.88938157+02	92	142.922722	97.429134	.89117351+02
82	134.097916	-52.194182	.88938158+02	93	142.922722	-142.570856	.89117350+02

Total Coulomb Energy: 4448.35063433

## 101 POINTS

D<sub>3</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
11	39.933973	30.013143	.89805563+02	72	116.950830	-88.834742	.89890498+02
89	140.064177	-169.153505	.89805581+02	29	63.048047	-170.306889	.89890508+02
91	140.066786	70.846290	.89805587+02	95	157.388704	-142.653370	.89893823+02
13	39.934646	-89.987062	.89805598+02	6	22.610639	3.506950	.89893897+02
90	140.066240	-49.155383	.89805624+02	7	22.610666	-116.489886	.89893888+02
12	39.934160	150.012339	.89805638+02	96	157.389463	97.354438	.89893898+02
1	.000000	-53.854128	.89812286+02	5	22.609137	123.511717	.89894079+02
101	179.999998	-179.429419	.89812282+02	97	157.391396	-22.654053	.89894135+02
74	119.272578	-158.463791	.89825273+02	98	158.531908	161.291737	.89913763+02
27	60.726020	-100.677266	.89825297+02	4	21.467350	-60.432538	.89913818+02
28	60.726059	139.321547	.89825295+02	2	21.466481	59.564768	.89913953+02
26	60.725514	19.321690	.89825318+02	99	158.533234	-78.713096	.89913992+02
75	119.274570	-38.463326	.89825309+02	3	21.466573	179.570211	.89914021+02
76	119.275256	81.537012	.89825324+02	100	158.534431	41.294762	.89914028+02
32	66.990899	114.907104	.89847575+02	22	56.494235	-27.386986	.89926881+02
68	113.007751	-134.049849	.89847578+02	80	123.505077	128.246317	.89926880+02
70	113.009737	-14.049199	.89847586+02	21	56.493452	-147.387667	.89926914+02
33	66.991347	-125.090734	.89847604+02	81	123.506756	-111.753631	.89926918+02
34	66.991765	-5.090663	.89847607+02	20	56.491094	92.611428	.89926941+02
69	113.008524	105.949228	.89847616+02	82	123.509418	8.246436	.89926941+02
24	59.777362	164.459175	.89860510+02	40	78.153034	153.212624	.89932331+02
78	120.222946	-63.601269	.89860511+02	62	101.845799	-172.355345	.89932352+02
77	120.221030	176.398726	.89860527+02	63	101.847618	-52.353774	.89932375+02
23	59.776546	44.460287	.89860548+02	39	78.152472	-86.785700	.89932415+02
25	59.777735	-75.539138	.89860560+02	38	78.151329	33.212584	.89932491+02
79	120.224346	56.398092	.89860577+02	64	101.849713	67.645504	.89932508+02
59	99.726421	166.559269	.89866721+02	15	43.426101	61.564054	.89978621+02
41	80.272050	174.297916	.89866746+02	87	136.574003	-80.705244	.89978643+02
43	80.273020	-65.700612	.89866743+02	88	136.574848	39.294755	.89978662+02
60	99.727529	-73.438597	.89866774+02	14	43.425512	-178.438063	.89978685+02
42	80.272886	54.296760	.89866807+02	16	43.426428	-58.437423	.89978685+02
61	99.728061	46.561159	.89866801+02	86	136.573057	159.297764	.89978678+02
52	90.001858	-9.569256	.89868967+02	35	76.715761	94.582018	.89995016+02
50	89.998079	110.427195	.89868978+02	67	103.284646	6.275528	.89995010+02
51	90.000082	-129.569994	.89869001+02	37	76.718716	-25.413122	.89995063+02
44	81.121908	130.730297	.89872093+02	66	103.282516	-113.725482	.89995087+02
56	98.876698	-149.872864	.89872090+02	65	103.280860	126.271129	.89995099+02
45	81.122598	-109.268067	.89872100+02	36	76.717536	-145.414164	.89995121+02
46	81.123519	10.731074	.89872107+02	55	97.087335	145.770782	.90057220+02
58	98.878204	-29.871722	.89872099+02	48	82.913201	-44.912525	.90057234+02
57	98.877090	90.127157	.89872109+02	47	82.911765	-164.913727	.90057270+02
17	46.148379	.000000	.89883721+02	53	97.086137	25.773915	.90057313+02
83	133.850084	-139.142090	.89883722+02	54	97.086560	-94.226425	.90057307+02
84	133.851944	100.859675	.89883719+02	49	82.914957	75.083879	.90057334+02
19	46.148718	-119.999565	.89883732+02	92	143.507250	129.088175	.90107666+02
18	46.148403	120.000311	.89883780+02	10	36.491919	-28.227798	.90107700+02
85	133.852482	-19.142482	.89883786+02	9	36.491397	-148.226702	.90107730+02
30	63.049233	-50.305469	.89890473+02	93	143.508877	-110.916336	.90107741+02
31	63.049983	69.693370	.89890474+02	8	36.488714	91.774064	.90107839+02
71	116.950806	151.164934	.89890481+02	94	143.511868	9.084441	.90107856+02
73	116.951052	31.164677	.89890475+02				

Total Coulomb Energy: 4540.59005175

## 102 POINTS

D<sub>3</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
33	69.102558	-172.905363	.90755101+02	24	57.120498	-152.160192	.90826416+02
31	69.101729	-52.906601	.90755116+02	79	122.879059	-27.840147	.90826421+02
72	110.898436	-127.095411	.90755106+02	81	122.880591	-147.840763	.90826417+02
32	69.101944	67.094444	.90755121+02	5	25.083728	-65.192765	.90833077+02
70	110.897141	-7.094784	.90755120+02	98	154.916519	125.189385	.90833073+02
71	110.898192	112.905193	.90755113+02	4	25.083246	54.808352	.90833093+02
43	79.701126	28.066644	.90773443+02	6	25.083729	174.808352	.90833085+02
44	79.701883	148.067200	.90773456+02	97	154.915548	5.191676	.90833084+02
58	100.297496	31.932628	.90773446+02	99	154.917215	-114.807527	.90833086+02
60	100.298768	-88.067847	.90773450+02	16	47.779989	-55.755211	.90860088+02
45	79.702510	-91.933558	.90773466+02	86	132.220024	115.753310	.90860084+02
59	100.298194	151.932398	.90773468+02	18	47.780753	-175.753862	.90860105+02
10	35.615558	-28.484343	.90799785+02	87	132.220182	-124.246695	.90860115+02
92	144.383938	88.482070	.90799785+02	17	47.780273	64.246628	.90860129+02
11	35.615753	91.516424	.90799797+02	85	132.218773	-4.246682	.90860119+02
91	144.383566	-31.515935	.90799789+02	25	58.812342	19.171064	.90862584+02
12	35.616051	-148.484333	.90799802+02	26	58.813209	139.171215	.90862576+02
93	144.385120	-151.516403	.90799802+02	27	58.813982	-100.829760	.90862581+02
46	84.059090	49.171226	.90805644+02	76	121.186296	40.828059	.90862583+02
55	95.939641	10.828166	.90805642+02	77	121.186838	160.828379	.90862578+02
47	84.059256	169.171671	.90805661+02	78	121.187314	-79.171488	.90862576+02
48	84.059490	-70.829268	.90805657+02	51	89.905684	-169.853622	.90873588+02
56	95.940939	130.828161	.90805661+02	54	90.095402	-130.147333	.90873590+02
57	95.941576	-109.172500	.90805660+02	50	89.904759	70.146009	.90873615+02
30	63.858881	-75.778116	.90807942+02	49	89.904716	-49.854666	.90873626+02
74	116.141620	135.776663	.90807943+02	52	90.094370	-10.146605	.90873621+02
28	63.858521	44.222890	.90807955+02	53	90.095073	109.853690	.90873622+02
29	63.858785	164.222992	.90807955+02	9	32.266744	8.971535	.90930802+02
73	116.140230	15.776573	.90807949+02	94	147.732328	51.026841	.90930805+02
75	116.141954	-104.223532	.90807959+02	95	147.733166	-68.970872	.90930807+02
63	100.466735	-147.917740	.90815682+02	8	32.266689	128.971811	.90930818+02
41	79.534062	87.916676	.90815694+02	7	32.266327	-111.029210	.90930840+02
42	79.534398	-152.083254	.90815685+02	96	147.734739	171.027365	.90930839+02
61	100.465242	-27.917083	.90815698+02	37	75.541631	6.913599	.90945911+02
40	79.533737	-32.084349	.90815712+02	38	75.542884	126.914423	.90945925+02
62	100.465816	92.083223	.90815711+02	64	104.457086	53.085520	.90945918+02
3	12.550316	-8.554400	.90817139+02	66	104.457500	-66.914893	.90945916+02
100	167.448957	68.549599	.90817137+02	39	75.543767	-113.086287	.90945949+02
101	167.449310	-51.442555	.90817152+02	65	104.457123	173.085098	.90945949+02
1	12.550004	-128.554188	.90817171+02	35	69.457032	-133.418610	.91021953+02
2	12.550200	111.446924	.90817165+02	69	110.544095	-166.582554	.91021947+02
102	167.451200	-171.447901	.90817171+02	36	69.457192	106.581506	.91021962+02
19	50.796241	-4.395464	.90823612+02	67	110.542357	-46.581616	.91021966+02
20	50.796244	-124.394826	.90823607+02	34	69.456794	-13.419875	.91021979+02
21	50.796405	115.605426	.90823605+02	68	110.542529	73.418621	.91021977+02
82	129.202944	64.393939	.90823611+02	15	43.700509	-83.786185	.91025896+02
83	129.203264	-55.605149	.90823605+02	89	136.300116	143.784317	.91025891+02
84	129.204893	-175.606459	.90823603+02	14	43.700247	156.215651	.91025923+02
22	57.119754	-32.161274	.90826416+02	88	136.298872	23.783339	.91025936+02
80	122.879818	92.159698	.90826415+02	90	136.300411	-96.215835	.91025935+02
23	57.120275	87.840155	.90826425+02	13	43.699832	36.216196	.91025949+02

Total Coulomb Energy: 4633.73656590

## 103 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
25	58.731165	-35.139920	.91692275+02	24	56.839714	-8.608070	.91777803+02
26	58.793194	144.744986	.91692275+02	33	68.388637	-123.066826	.91781220+02
103	179.900169	-107.099503	.91705932+02	34	68.580586	56.954809	.91781219+02
51	90.818520	-126.811958	.91713441+02	1	10.204692	-116.590138	.91787250+02
52	91.006462	53.186963	.91713442+02	2	10.401660	63.589326	.91787250+02
21	53.170055	-140.097004	.91715723+02	85	134.377102	-135.365294	.91787523+02
22	53.337566	39.984093	.91715723+02	86	134.552862	44.541761	.91787523+02
77	119.330780	-37.123255	.91719817+02	93	142.110237	-164.530043	.91790088+02
78	119.398980	142.982309	.91719817+02	94	142.217400	15.253074	.91790088+02
91	140.182383	-48.978723	.91723193+02	79	120.773010	-61.259449	.91797226+02
92	140.287527	131.225224	.91723193+02	80	120.911995	118.826119	.91797226+02
69	112.471052	-128.994040	.91723957+02	17	47.848377	-112.653946	.91800546+02
70	112.656273	50.975001	.91723957+02	18	48.047089	67.363470	.91800546+02
27	63.240258	-59.136408	.91733065+02	35	73.612537	-80.252328	.91803915+02
30	63.374046	120.789086	.91733065+02	36	73.790692	99.721323	.91803915+02
39	76.077158	-142.970963	.91734071+02	66	104.081685	-169.367170	.91805081+02
42	76.238962	37.057848	.91734070+02	67	104.174519	10.588337	.91805081+02
7	31.429803	-91.683610	.91735742+02	28	63.246289	-161.724285	.91807629+02
8	31.622313	88.230134	.91735742+02	29	63.361977	18.357535	.91807629+02
57	96.594612	-28.957167	.91745879+02	75	118.902514	-151.908443	.91810248+02
58	96.635606	151.065487	.91745879+02	76	119.044053	28.013598	.91810249+02
19	51.216021	-81.232369	.91749961+02	55	94.015473	172.559879	.91822893+02
20	51.395725	98.697958	.91749961+02	56	94.048931	-7.453990	.91822893+02
43	79.413256	-42.582637	.91751082+02	11	39.517570	-22.619568	.91830487+02
44	79.499213	137.383823	.91751082+02	12	39.537207	157.139654	.91830487+02
15	43.198043	-166.947464	.91753930+02	83	124.964377	-109.155818	.91838321+02
16	43.298590	13.235896	.91753930+02	84	125.163898	70.839140	.91838321+02
53	92.354498	-88.745579	.91756385+02	71	113.095211	164.850515	.91840484+02
54	92.543988	91.257101	.91756385+02	72	113.101845	-15.234573	.91840483+02
9	31.970467	-134.088350	.91758503+02	101	159.330698	-140.094002	.91840828+02
10	32.148480	46.055971	.91758502+02	102	159.497883	39.615389	.91840829+02
97	156.565966	-18.201272	.91761668+02	47	84.169122	-62.785669	.91895319+02
98	156.569010	162.259329	.91761667+02	48	84.311996	117.200268	.91895319+02
73	115.017121	-87.974086	.91762558+02	49	85.214702	-162.166111	.91896336+02
74	115.205733	92.056587	.91762558+02	50	85.329038	17.847418	.91896335+02
40	76.122516	-21.584441	.91764071+02	3	21.886899	-49.608828	.91904587+02
41	76.138224	158.366419	.91764071+02	4	21.994820	129.974209	.91904587+02
99	158.200054	-72.721608	.91764915+02	45	83.545473	-107.189919	.91905537+02
100	158.364555	107.562435	.91764915+02	46	83.745119	72.810107	.91905538+02
89	135.456656	-18.592475	.91765246+02	63	102.424653	-70.944923	.91941276+02
90	135.461514	161.610334	.91765246+02	64	102.585825	109.081199	.91941276+02
59	98.564175	-146.323536	.91765808+02	5	23.329428	-176.167595	.91953318+02
60	98.718809	33.657267	.91765808+02	6	23.401443	4.263416	.91953318+02
13	42.463646	-55.272438	.91769314+02	31	65.006053	-99.615246	.91953401+02
14	42.587278	124.556642	.91769314+02	32	65.204006	80.372698	.91953400+02
61	101.230053	-49.001137	.91770293+02	81	123.659361	-175.552193	.91954434+02
62	101.335519	131.032675	.91770293+02	82	123.732490	4.323938	.91954434+02
65	104.045497	-108.074066	.91774158+02	37	75.348844	179.955395	.91979939+02
68	104.245116	71.925072	.91774158+02	38	75.407461	.005181	.91979939+02
87	135.121368	-80.251147	.91777364+02	95	145.341192	-107.954911	.91995548+02
88	135.299433	99.839811	.91777363+02	96	145.540825	72.040729	.91995548+02
23	56.810472	171.262823	.91777802+02				

Total Coulomb Energy: 4727.83661683



## 104 POINTS

D<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
51	88.925764	168.089081	.92635334+02	45	84.330985	-33.507502	.92732635+02
52	88.925830	-11.910382	.92635332+02	46	84.347487	146.488642	.92732642+02
53	91.066539	-171.195536	.92635347+02	58	95.646958	-149.595667	.92732702+02
54	91.082631	8.803347	.92635346+02	60	95.677611	30.400675	.92732705+02
7	30.622213	-171.333706	.92654453+02	99	150.823946	-111.571966	.92741026+02
8	30.638351	8.738200	.92654451+02	100	150.868450	68.414654	.92741025+02
97	149.371307	168.235172	.92654482+02	5	29.133494	-71.502523	.92741079+02
98	149.371601	-11.841020	.92654485+02	6	29.172692	108.456192	.92741079+02
49	87.764855	-81.224009	.92661519+02	27	60.446526	-137.095093	.92745828+02
50	87.807221	98.775363	.92661522+02	28	60.483846	42.919561	.92745824+02
55	92.189104	-101.879439	.92661524+02	77	119.525093	-46.027681	.92745867+02
56	92.234351	78.120557	.92661524+02	78	119.550178	133.993662	.92745859+02
37	71.124842	-94.421341	.92669958+02	25	55.749100	-113.300872	.92759867+02
38	71.169769	85.576496	.92669955+02	26	55.793566	66.705073	.92759869+02
67	108.829088	-88.684551	.92669983+02	79	124.207992	-69.815234	.92759860+02
68	108.873111	91.319111	.92669978+02	80	124.246257	110.201252	.92759860+02
35	70.609519	-178.303225	.92670740+02	95	147.575008	-152.201077	.92763227+02
36	70.620262	1.712012	.92670733+02	96	147.603872	27.744395	.92763226+02
69	109.382810	175.197565	.92670794+02	9	32.401928	-30.837744	.92763255+02
70	109.388503	-4.818488	.92670799+02	10	32.416710	149.094437	.92763254+02
23	53.837850	-161.468803	.92690413+02	85	129.001451	-96.543874	.92766854+02
24	53.860976	18.559684	.92690411+02	86	129.046452	83.459666	.92766854+02
81	126.148073	-21.665165	.92690443+02	19	50.953520	-86.556719	.92766865+02
82	126.155543	158.367449	.92690439+02	20	50.997253	93.433458	.92766865+02
103	168.649769	-148.979937	.92698623+02	13	39.985938	-139.617733	.92775415+02
104	168.680544	30.855530	.92698619+02	14	40.022055	40.415302	.92775413+02
1	11.325777	-33.936829	.92698677+02	91	139.986464	-43.524078	.92775477+02
2	11.342865	145.852901	.92698672+02	92	140.009907	136.521856	.92775472+02
39	74.638580	-157.062204	.92703731+02	33	69.069851	-19.920789	.92782519+02
40	74.664603	22.947766	.92703725+02	34	69.076068	160.062351	.92782528+02
65	105.344086	-26.054840	.92703771+02	71	110.916932	-163.169605	.92782620+02
66	105.354993	153.957430	.92703768+02	72	110.938826	16.814934	.92782627+02
17	49.607482	173.488564	.92708582+02	41	75.663384	-115.735381	.92792931+02
18	49.611886	-6.473048	.92708580+02	42	75.707388	64.267161	.92792929+02
87	130.385538	-176.592176	.92708577+02	63	104.294390	-67.375284	.92792989+02
88	130.397636	3.370708	.92708579+02	64	104.331632	112.631455	.92792986+02
89	131.401203	-123.857514	.92716544+02	47	84.355449	-59.789022	.92837226+02
90	131.443085	56.127622	.92716542+02	48	84.388998	120.207940	.92837237+02
15	48.560222	-59.224956	.92716574+02	57	95.605853	-123.311211	.92837314+02
16	48.593638	120.747907	.92716570+02	59	95.648047	56.687201	.92837322+02
29	67.461643	-71.596581	.92717573+02	43	80.346718	-136.581383	.92915773+02
30	67.500760	108.393842	.92717576+02	44	80.384279	43.422747	.92915768+02
75	112.495841	-111.500870	.92717617+02	61	99.624921	-46.530172	.92915804+02
76	112.540464	68.496086	.92717617+02	62	99.650319	133.476393	.92915799+02
101	162.534004	-56.013509	.92725429+02	83	127.554407	-150.098129	.92919791+02
102	162.565279	124.090145	.92725429+02	84	127.584507	29.875981	.92919788+02
3	17.430256	-127.176935	.92725451+02	21	52.420549	-32.975380	.92919823+02
4	17.471406	52.884364	.92725452+02	22	52.436937	146.992067	.92919820+02
73	111.551076	-135.956419	.92731262+02	93	144.043257	-75.816236	.92945758+02
74	111.588502	44.033527	.92731259+02	94	144.083801	104.211381	.92945762+02
31	68.415343	-47.134758	.92731294+02	11	35.912461	-107.303226	.92945799+02
32	68.441563	132.850636	.92731293+02	12	35.957631	72.702529	.92945804+02

Total Coulomb Energy: 4822.92698787

105 POINTS  
C<sub>2</sub> (NONMIN)

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
16	43.141973	-148.565090	.93591043+02	93	141.069855	-35.842275	.93672636+02
17	43.141974	31.434894	.93591043+02	84	128.771423	-89.094255	.93673392+02
20	52.856387	-96.152018	.93591163+02	85	128.771425	90.905764	.93673393+02
21	52.856390	83.847961	.93591163+02	26	58.186280	-122.085785	.93680591+02
98	150.690277	-179.999990	.93604603+02	27	58.186280	57.914192	.93680590+02
99	150.690306	.000021	.93604602+02	36	72.250811	174.482574	.93688193+02
44	78.553104	-128.492329	.93608036+02	37	72.250835	-5.517432	.93688193+02
45	78.553105	51.507657	.93608036+02	32	71.130506	-84.587681	.93689316+02
96	145.016792	-142.582720	.93612487+02	33	71.130512	95.412301	.93689316+02
97	145.016808	37.417309	.93612486+02	52	90.844050	-70.418208	.93696003+02
14	42.057328	136.323278	.93612950+02	53	90.844050	109.581780	.93696003+02
15	42.057335	-43.676693	.93612950+02	62	99.340678	-134.120155	.93703219+02
50	90.511262	-91.334940	.93613839+02	63	99.340683	45.879840	.93703219+02
51	90.511266	88.665047	.93613839+02	68	109.806245	-76.618673	.93706776+02
66	106.661769	-154.217051	.93620801+02	69	109.806245	103.381328	.93706776+02
67	106.661787	25.782951	.93620802+02	72	111.259498	-175.082895	.93711255+02
42	77.618590	153.146145	.93621250+02	73	111.259524	4.917103	.93711255+02
43	77.618608	-26.853853	.93621250+02	60	98.453107	147.566624	.93715341+02
40	73.141241	-106.227368	.93621529+02	61	98.453128	-32.433376	.93715340+02
41	73.141241	73.772614	.93621529+02	12	38.495521	61.985772	.93715642+02
64	104.698035	126.190056	.93624732+02	13	38.495522	-118.014212	.93715642+02
65	104.698049	-53.809944	.93624732+02	90	132.760836	-115.408041	.93725858+02
104	168.461723	-141.630194	.93629064+02	91	132.760836	64.591979	.93725858+02
105	168.461740	38.369911	.93629064+02	82	124.825613	119.290378	.93725937+02
86	129.515829	-163.549637	.93635920+02	83	124.825626	-60.709639	.93725937+02
87	129.515852	16.450369	.93635920+02	88	130.876463	169.710590	.93730063+02
54	91.170181	-170.131306	.93636533+02	89	130.876492	-10.289412	.93730063+02
55	91.170207	9.868689	.93636533+02	8	34.954296	-78.222455	.93734499+02
18	52.670311	-172.645424	.93641058+02	9	34.954298	101.777525	.93734499+02
19	52.670333	7.354575	.93641058+02	10	37.163573	169.317526	.93737369+02
24	56.455184	159.812775	.93642357+02	11	37.163583	-10.682455	.93737369+02
25	56.455196	-20.187212	.93642357+02	46	84.809532	132.664974	.93752698+02
58	92.679057	-112.713943	.93648860+02	47	84.809545	-47.335020	.93752698+02
59	92.679058	67.286048	.93648860+02	100	151.914368	76.040532	.93753674+02
80	122.655893	-139.929462	.93650055+02	101	151.914370	-103.959510	.93753674+02
81	122.655907	40.070545	.93650055+02	22	53.349600	-68.487568	.93754127+02
30	63.186917	-144.665030	.93657575+02	23	53.349603	111.512408	.93754127+02
31	63.186922	35.334950	.93657575+02	70	109.852880	-98.269567	.93762545+02
4	21.085529	139.976665	.93660123+02	71	109.852888	81.730431	.93762545+02
5	21.085537	-40.023321	.93660123+02	1	.000003	-51.480789	.93797136+02
56	92.069592	169.313208	.93661140+02	34	71.397394	-164.410666	.93836857+02
57	92.069619	-10.686796	.93661140+02	35	71.397419	15.589323	.93836857+02
78	120.250986	142.916025	.93664844+02	76	113.065255	-119.111185	.93860257+02
79	120.251011	-37.083985	.93664843+02	77	113.065256	60.888812	.93860258+02
28	62.747591	136.867283	.93665893+02	94	143.911854	110.879080	.93877205+02
29	62.747599	-43.132700	.93665893+02	95	143.911861	-69.120955	.93877204+02
6	23.900625	19.251331	.93666723+02	74	111.555924	163.521179	.93894017+02
7	23.900627	-160.748663	.93666723+02	75	111.555953	-16.478825	.93894017+02
102	162.560181	131.991081	.93668997+02	2	19.605600	73.577630	.93939522+02
103	162.560202	-48.008970	.93668997+02	3	19.605601	-106.422363	.93939521+02
48	85.379527	-149.034349	.93669964+02	38	72.403108	-63.148499	.93941776+02
49	85.379540	30.965644	.93669964+02	39	72.403108	116.851485	.93941776+02
92	141.069828	144.157742	.93672636+02				

Total Coulomb Energy: 4919.09887396

105 POINTS  
No Symmetry

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
79	117.719559	-87.345322	.93550033+02	89	133.659704	50.549672	.93679318+02
44	78.703830	130.650885	.93583189+02	72	113.160295	37.612543	.93680265+02
26	58.738139	121.980710	.93590741+02	46	80.663163	152.050728	.93681421+02
6	70.856992	28.060839	.93592234+02	70	110.264242	-127.450201	.93682586+02
53	89.929871	-125.839843	.93596114+02	95	146.064514	-160.692562	.93683039+02
78	117.152456	123.379478	.93599520+02	86	129.514162	23.062152	.93690074+02
58	96.525723	-87.374657	.93604120+02	27	60.895263	-20.210897	.93695722+02
98	149.280714	73.001334	.93604236+02	9	31.047645	-140.110481	.93696216+02
105	170.628710	50.527143	.93606845+02	13	40.579323	108.213522	.93702250+02
8	28.286962	-97.320304	.93608792+02	80	117.979068	147.356716	.93704306+02
35	69.996772	170.586981	.93610165+02	93	138.859861	-4.881097	.93704605+02
68	106.328938	-67.144496	.93610629+02	90	133.711016	-33.905739	.93705076+02
3	18.424026	-48.549518	.93610926+02	10	35.352574	43.798954	.93705188+02
2	10.439706	-142.739698	.93614354+02	5	27.475732	6.884924	.93706002+02
76	115.397943	100.937618	.93615078+02	83	126.442780	-167.534569	.93706200+02
61	97.242361	-27.169523	.93616658+02	87	131.534533	-137.142780	.93708608+02
14	40.826831	140.265507	.93617246+02	92	136.228445	134.702209	.93710215+02
84	126.511621	-111.186593	.93619188+02	22	54.254447	-142.708826	.93711286+02
91	136.165483	105.407610	.93620062+02	37	74.255759	-146.482781	.93712101+02
40	76.588875	109.570684	.93620257+02	67	105.860255	17.212872	.93713819+02
99	150.461401	28.816451	.93621484+02	33	67.464432	69.046714	.93714129+02
74	114.165185	-44.404502	.93622481+02	7	28.159297	173.307976	.93715772+02
49	85.895535	11.126985	.93626907+02	102	157.490625	-18.619304	.93728664+02
59	96.938959	116.328597	.93636547+02	43	77.737621	-32.611256	.93728867+02
29	61.520304	145.869957	.93637985+02	1	10.319493	42.979034	.93728979+02
48	85.208606	-105.913249	.93638358+02	11	37.743635	-29.730291	.93729788+02
97	149.239710	-120.641522	.93639862+02	69	106.636630	79.935315	.93731055+02
66	105.625522	-106.707229	.93640187+02	19	49.187420	-89.476836	.93736886+02
45	80.499442	-11.248727	.93640573+02	4	20.111768	127.699916	.93737897+02
51	88.799613	70.385965	.93640758+02	50	85.961494	-69.222064	.93738589+02
85	128.545652	79.834235	.93643615+02	104	167.440376	-166.654694	.93741711+02
25	58.611082	95.929539	.93643789+02	65	103.481276	-167.361296	.93743775+02
56	94.555105	-48.424537	.93647071+02	77	116.492778	-21.116364	.93748556+02
18	47.716720	73.921840	.93656702+02	47	83.469824	-165.661764	.93750906+02
94	139.089920	-89.236243	.93658996+02	21	50.681246	23.518852	.93753758+02
12	39.386594	-63.215736	.93659632+02	71	112.156096	173.491343	.93765409+02
41	76.941476	49.402400	.93661197+02	57	94.743526	96.311007	.93767044+02
82	126.421607	-64.015931	.93662704+02	88	131.558807	166.546494	.93772923+02
63	99.634277	-5.307175	.93662856+02	103	163.575323	-82.396996	.93780019+02
54	91.118821	32.132217	.93664744+02	60	96.982410	52.130961	.93795525+02
28	61.022513	-69.404492	.93666098+02	42	77.129471	87.594812	.93809700+02
39	74.562569	-86.187369	.93667440+02	75	115.128255	60.710556	.93819650+02
24	56.327504	48.349761	.93668476+02	31	64.763217	-104.844623	.93843526+02
32	66.574843	5.058091	.93674143+02	38	74.265865	-52.858734	.93874573+02
62	98.643690	136.485071	.93677018+02	81	119.405046	1.266836	.93875351+02
30	63.974032	-168.018515	.93677089+02	6	27.974803	79.465265	.93880393+02
23	55.686139	-43.838917	.93677440+02	96	146.237200	-57.487212	.93884813+02
55	94.175856	-145.923950	.93677495+02	64	99.733972	157.119907	.93885767+02
52	89.553008	174.904282	.93677679+02	73	114.006726	-148.925606	.93888519+02
34	69.705946	-125.567904	.93677715+02	15	44.417866	-166.095669	.93890400+02
20	50.100416	167.066414	.93678440+02	17	46.942111	-2.531850	.93898122+02
16	46.815476	-118.057000	.93678778+02	100	150.627855	160.156263	.93899593+02
101	156.751928	115.477466	.93678792+01				

Total Coulomb Energy: 4919.05619731

## 106 POINTS

D<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
53	89.989052	-179.989836	.94529615+02	103	162.507256	123.174755	.94619130+02
54	90.018659	.009513	.94529620+02	64	101.111646	-144.451424	.94626198+02
9	34.476159	152.661427	.94532684+02	63	101.082167	35.565470	.94626222+02
10	34.544007	-27.436010	.94532676+02	43	78.874468	144.469711	.94626586+02
97	145.486849	27.466848	.94532849+02	44	78.951733	-35.541389	.94626604+02
98	145.502699	-152.671236	.94532862+02	86	129.108326	-97.939157	.94628835+02
7	29.592301	-169.804514	.94532888+02	85	129.022631	82.095333	.94628861+02
8	29.605193	10.029214	.94532888+02	21	50.875897	97.922073	.94629107+02
99	150.380480	169.817095	.94533125+02	22	50.969272	-82.064337	.94629113+02
100	150.425903	-10.033547	.94533119+02	50	87.521935	-159.969606	.94636383+02
87	129.594555	-174.054808	.94553674+02	49	87.518125	20.025412	.94636398+02
88	129.614683	6.022293	.94553679+02	57	92.459715	159.990578	.94636457+02
19	50.380715	174.067335	.94553745+02	58	92.519250	-20.006632	.94636469+02
20	50.419365	-6.004617	.94553745+02	45	81.581785	42.925015	.94642914+02
51	88.858849	100.422667	.94564861+02	46	81.622259	-137.061907	.94642914+02
52	88.952884	-79.576770	.94564856+02	61	98.358787	137.077421	.94642950+02
55	91.036438	79.591583	.94564989+02	62	98.442751	-42.916025	.94642956+02
56	91.119706	-100.408909	.94565005+02	89	130.372267	159.740135	.94663198+02
2	11.502180	-28.080328	.94570237+02	90	130.432083	-20.196329	.94663207+02
1	11.433720	152.247299	.94570250+02	17	49.600627	20.197016	.94663328+02
105	168.528162	28.145478	.94570352+02	18	49.604662	-159.722097	.94663329+02
106	168.544838	-152.321945	.94570374+02	83	124.669423	108.985258	.94669937+02
67	108.014971	-164.935946	.94577049+02	84	124.765118	-71.014404	.94669928+02
68	108.019727	15.094456	.94577042+02	23	55.237425	70.998363	.94669978+02
39	71.963792	164.950596	.94577157+02	24	55.313539	-108.961924	.94669988+02
40	72.016289	-15.075633	.94577147+02	15	46.223930	124.475150	.94674602+02
81	123.785475	30.256248	.94596679+02	16	46.315527	-55.550285	.94674595+02
82	123.805874	-149.805708	.94596673+02	91	133.708279	55.590814	.94674785+02
25	56.173166	149.816206	.94596909+02	92	133.767401	-124.481812	.94674810+02
26	56.244389	-30.225859	.94596908+02	59	94.877046	58.359748	.94693780+02
37	71.331834	85.889512	.94601618+02	60	94.938979	-121.646215	.94693775+02
38	71.419646	-94.097922	.94601621+02	47	85.043406	121.657060	.94693870+02
69	108.563162	94.123590	.94601770+02	48	85.136132	-58.344813	.94693861+02
70	108.655366	-85.883744	.94601791+02	6	27.581201	-67.092423	.94704248+02
71	110.620601	174.355383	.94605533+02	5	27.486070	112.923377	.94704269+02
72	110.659296	-5.612167	.94605532+02	101	152.435425	67.160879	.94704515+02
35	69.357733	-174.340149	.94605608+02	102	152.508423	-112.959526	.94704544+02
36	69.377926	5.624372	.94605607+02	34	69.070714	-72.691876	.94732185+02
41	75.130112	63.982194	.94607323+02	33	68.975957	107.307076	.94732200+02
42	75.198714	-116.000007	.94607316+02	73	110.922538	72.724115	.94732627+02
79	120.301114	132.556868	.94607390+02	74	110.999806	-107.296165	.94732662+02
80	120.388747	-47.420594	.94607385+02	78	114.424551	-128.762831	.94815690+02
27	59.632040	47.413225	.94607429+02	77	114.371435	51.272110	.94815723+02
28	59.679098	-132.538065	.94607434+02	29	65.564339	128.780418	.94816171+02
65	104.783082	116.018464	.94607557+02	30	65.653655	-51.234215	.94816186+02
66	104.877751	-63.978017	.94607559+02	75	111.423256	152.817789	.94826212+02
93	140.823751	134.752136	.94614624+02	76	111.491834	-27.156355	.94826216+02
94	140.909790	-45.195441	.94614614+02	31	68.540627	27.160394	.94826370+02
13	39.109463	45.169940	.94614790+02	32	68.556074	-152.802319	.94826374+02
14	39.153314	-134.726311	.94614795+02	96	144.156744	-77.966147	.94827301+02
3	17.409656	56.668521	.94619002+02	95	144.061590	102.048455	.94827332+02
4	17.469424	-123.095209	.94619011+02	11	35.839950	77.925097	.94827608+02
104	162.599916	-56.744973	.94619108+02	12	35.922337	-102.009585	.94827619+02

Total Coulomb Energy: 5015.98459608

## 107 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
4	21.424096	-121.672315	.95440937+02	2	20.121875	120.702251	.95578842+02
5	21.424114	58.327680	.95440935+02	3	20.121879	-59.297708	.95578842+02
6	22.316621	178.890623	.95463405+02	32	66.837633	-119.830034	.95579843+02
7	22.316632	-1.109344	.95463404+02	33	66.837650	60.169991	.95579843+02
78	116.048890	-45.552553	.95475417+02	22	56.257462	-73.713500	.95585809+02
79	116.048903	134.447454	.95475417+02	23	56.257466	106.286499	.95585810+02
82	121.302953	-23.262736	.95484594+02	74	114.775263	-88.429383	.95586372+02
83	121.302977	156.737274	.95484594+02	75	114.775298	91.570617	.95586372+02
52	88.480071	-124.734206	.95490074+02	98	148.544521	-114.677234	.95594004+02
53	88.480089	55.265815	.95490075+02	99	148.544544	65.322728	.95594005+02
106	169.980650	-108.447758	.95490518+02	36	73.077217	119.863334	.95594198+02
107	169.980661	71.552115	.95490519+02	37	73.077218	-60.136656	.95594197+02
28	60.383225	-22.619391	.95494464+02	46	80.954467	-160.946259	.95596079+02
29	60.383233	157.380606	.95494461+02	47	80.954468	19.053766	.95596081+02
1	.000000	10.550452	.95496610+02	38	73.984829	-84.455417	.95599941+02
26	57.951428	-99.073599	.95497138+02	39	73.984845	95.544585	.95599942+02
27	57.951442	80.926412	.95497138+02	10	37.214987	-89.522567	.95606298+02
94	138.322561	-40.436337	.95503369+02	11	37.214998	90.477433	.95606298+02
95	138.322582	139.563690	.95503370+02	86	129.253223	-65.395790	.95611021+02
62	99.730531	-31.235496	.95505917+02	87	129.253241	114.604231	.95611019+02
63	99.730542	148.764496	.95505916+02	68	103.618902	-11.227903	.95611544+02
104	160.013935	-24.881200	.95514567+02	69	103.618922	168.772085	.95611543+02
105	160.013960	155.118841	.95514567+02	70	109.276027	-67.384814	.95613604+02
42	77.958765	-39.044245	.95531769+02	71	109.276037	112.615186	.95613603+02
43	77.958767	140.955732	.95531769+02	16	43.010439	-118.679811	.95619223+02
72	109.475748	-129.530901	.95539196+02	17	43.010457	61.320199	.95619221+02
73	109.475767	50.469110	.95539197+02	76	115.925776	-150.845394	.95623809+02
8	37.105092	-152.136179	.95539429+02	77	115.925777	29.154609	.95623809+02
9	37.105110	27.863841	.95539428+02	40	75.438105	-140.821445	.95632118+02
18	46.182565	.255817	.95543336+02	41	75.438117	39.178579	.95632119+02
19	46.182568	-179.744184	.95543334+02	24	57.824543	134.534267	.95633413+02
44	80.501784	-104.718151	.95545085+02	25	57.824545	-45.465728	.95633414+02
45	80.501812	75.281865	.95545086+02	34	67.450258	-1.930429	.95634745+02
48	81.936204	-19.607947	.95550142+02	35	67.450274	178.069563	.95634742+02
49	81.211	160.392029	.95550140+02	102	153.566776	24.676858	.95639805+02
60	95.592546	-145.578083	.95552308+02	103	153.566776	-155.323071	.95639805+02
61	95.592555	34.421935	.95552308+02	30	60.479889	-160.961496	.95639821+02
56	94.791945	-50.838545	.95552790+02	31	60.479896	19.038510	.95639822+02
57	94.791956	129.161449	.95552790+02	84	122.354428	-111.278260	.95640361+02
96	140.052561	-9.768174	.95553563+02	85	122.354461	68.721737	.95640362+02
97	140.052584	170.231861	.95553563+02	58	95.035792	-89.635053	.95681712+02
100	151.442808	-70.248891	.95554116+02	59	95.035825	90.364959	.95681712+02
101	151.442833	109.751125	.95554117+02	92	134.936438	-91.325372	.95751324+02
80	119.817939	1.777249	.95560465+02	93	134.936474	88.674638	.95751324+02
81	119.817954	-178.222738	.95560465+02	90	134.188980	19.297390	.95761145+02
88	131.946640	-133.080986	.95560851+02	91	134.188990	-160.702578	.95761146+02
89	131.946659	46.918994	.95560852+02	54	89.700823	-70.636850	.95772384+02
12	38.974011	-26.524450	.95566291+02	55	89.700830	109.363153	.95772386+02
13	38.974013	153.475552	.95566289+02	50	87.330175	.000000	.95776833+02
66	102.376014	13.433814	.95566795+02	51	87.330192	179.999971	.95776831+02
67	102.376019	-166.566196	.95566794+02	20	55.256291	-138.922592	.95810464+02
64	101.939616	-108.883473	.95567476+02	21	55.256313	41.077423	.95810463+02
65	101.939646	71.116538	.95567477+02	14	40.122722	-57.404100	.95813829+02
				15	40.122722	122.595898	.95813828+02

Total Coulomb Energy: 5113.98085776

## 108 POINTS

C<sub>2</sub>

Index	Theta	Phi	Energy	Index	Theta	Phi	Energy
85	122.411922	40.033035	.96423926+02	15	44.634651	-57.274131	.96518708+02
86	122.411922	-139.966965	.96423926+02	16	44.634651	122.725869	.96518708+02
25	57.996638	-36.746390	.96425057+02	65	102.226257	-106.271810	.96521234+02
26	57.996638	143.253611	.96425057+02	66	102.226257	73.728190	.96521234+02
13	39.740570	9.700348	.96429128+02	95	140.513073	24.258715	.96522883+02
14	39.740570	-170.299652	.96429128+02	96	140.513073	-155.741285	.96522883+02
105	161.027260	39.264340	.96436030+02	63	100.093598	-49.065481	.96523974+02
106	161.027260	-140.735661	.96436029+02	64	100.093598	130.934519	.96523974+02
53	86.372681	-64.095320	.96436570+02	33	65.235658	55.231114	.96524513+02
54	86.372681	115.904679	.96436570+02	34	65.235658	-124.768886	.96524513+02
21	51.983063	-83.127530	.96438899+02	77	114.601740	-89.509531	.96525650+02
22	51.983063	96.872470	.96438899+02	78	114.601740	90.490469	.96525650+02
99	146.608490	-50.798746	.96441662+02	27	60.202552	13.256899	.96526637+02
100	146.608490	129.201254	.96441662+02	28	60.202552	-166.743101	.96526637+02
41	76.719168	-0.011041	.96451841+02	73	111.616979	-28.465377	.96530980+02
42	76.719168	179.988958	.96451841+02	74	111.616980	151.534622	.96530980+02
107	169.667696	-49.097020	.96458204+02	103	153.013620	90.676236	.96532345+02
108	169.667696	130.902977	.96458204+02	104	153.013620	-89.323763	.96532345+02
67	102.653523	29.880127	.96468728+02	1	10.043480	-99.793036	.96534724+02
68	102.653523	-150.119873	.96468728+02	2	10.043480	80.206964	.96534724+02
101	152.488514	-10.698969	.96484610+02	49	84.428611	-118.648140	.96541763+02
102	152.488514	169.301031	.96484610+02	50	84.428611	61.351860	.96541763+02
69	103.814201	51.658216	.96486179+02	97	141.082918	55.463364	.96549151+02
70	103.814201	-128.341784	.96486179+02	98	141.082918	-124.536635	.96549151+02
43	77.514990	-44.882489	.96490518+02	3	19.976821	.000000	.96550278+02
44	77.514990	135.117512	.96490517+02	4	19.976821	180.000000	.96550278+02
39	73.672940	-21.878874	.96499265+02	59	95.023425	-82.804288	.96550372+02
40	73.672940	158.121126	.96499265+02	60	95.023426	97.195712	.96550372+02
31	64.458529	-61.095515	.96499459+02	81	120.594199	-115.621655	.96561306+02
32	64.458529	118.904485	.96499459+02	82	120.594199	64.378345	.96561306+02
11	39.466046	-23.853366	.96500875+02	57	93.378058	-11.223353	.96567315+02
12	39.466046	156.146635	.96500875+02	58	93.378058	168.776648	.96567315+02
23	56.652741	-10.102581	.96502127+02	75	113.369061	-7.238656	.96570230+02
24	56.652741	169.897419	.96502127+02	76	113.369061	172.761343	.96570230+02
61	98.936255	8.610661	.96508193+02	29	64.294464	-102.315900	.96573835+02
62	98.936255	-171.389339	.96508193+02	30	64.294464	77.684100	.96573835+02
45	82.690928	19.825564	.96510169+02	89	132.437866	-28.549323	.96574787+02
46	82.690928	-160.174437	.96510169+02	90	132.437866	151.450676	.96574787+02
7	28.501622	-133.222366	.96510552+02	83	121.173553	-49.015501	.96578802+02
8	28.501622	46.777633	.96510552+02	84	121.173553	130.984499	.96578803+02
19	47.761815	37.407926	.96512215+02	51	85.787255	41.332608	.96598165+02
20	47.761815	-142.592073	.96512215+02	52	85.787255	-138.667393	.96598165+02
37	73.002791	-80.583262	.96512920+02	55	91.865670	-30.866338	.96704505+02
38	73.002791	99.416737	.96512920+02	56	91.865670	149.133661	.96704504+02
79	118.839845	16.551867	.96514200+02	47	83.557538	-98.775615	.96714625+02
80	118.839845	-163.448133	.96514199+02	48	83.557538	81.224385	.96714625+02
9	32.290824	-90.749661	.96514298+02	91	132.571703	-2.227635	.96720135+02
10	32.290824	89.250339	.96514298+02	92	132.571703	177.772366	.96720135+02
17	46.313873	-113.655874	.96517631+02	5	25.243099	-51.342454	.96727769+02
18	46.313873	66.344126	.96517631+02	6	25.243099	128.657545	.96727769+02
71	109.154387	-67.945559	.96517952+02	35	67.430223	33.733503	.96729158+02
72	109.154387	112.054441	.96517952+02	36	67.430223	-146.266497	.96729158+02
87	130.820549	-70.244841	.96518208+02	93	133.647846	-96.407621	.96730249+02
88	130.820549	109.755159	.96518208+02	94	133.647846	83.592378	.96730249+02

Total Coulomb Energy: 5212.81350783